National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

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HECC Deploys Pathfinding Systems for Future Roadmap

- In order to best meet future physics-based modeling and simulation requirements for the agency, HECC is investigating alternate architectures that could shape the project's processor architecture roadmap in the medium term.
- The Systems team deployed two systems that will be used to investigate ways to address the bottleneck between memory and processors.
  - Tfe2: The front-end system for all of the pathfinding systems. It consists of an AMD EPYC 7413 24-core processor; 256 gigabytes (GB) RAM; 1 terabyte (TB) /home and 16 TB /nobackupp filesystems.
  - Vector1 and Vector2: Two specialized compute nodes with NEC Vector Engines. Each node consists of two Intel Xeon Gold 6248R, 3.00 gigahertz, 24-core processors; 384 GB RAM; eight NEC Vector Engine Accelerators, each with 48 GB HBM2 stacked memory.
- HECC applications experts will use these systems to explore ways to best optimize application performance for the Vector Engine accelerators.

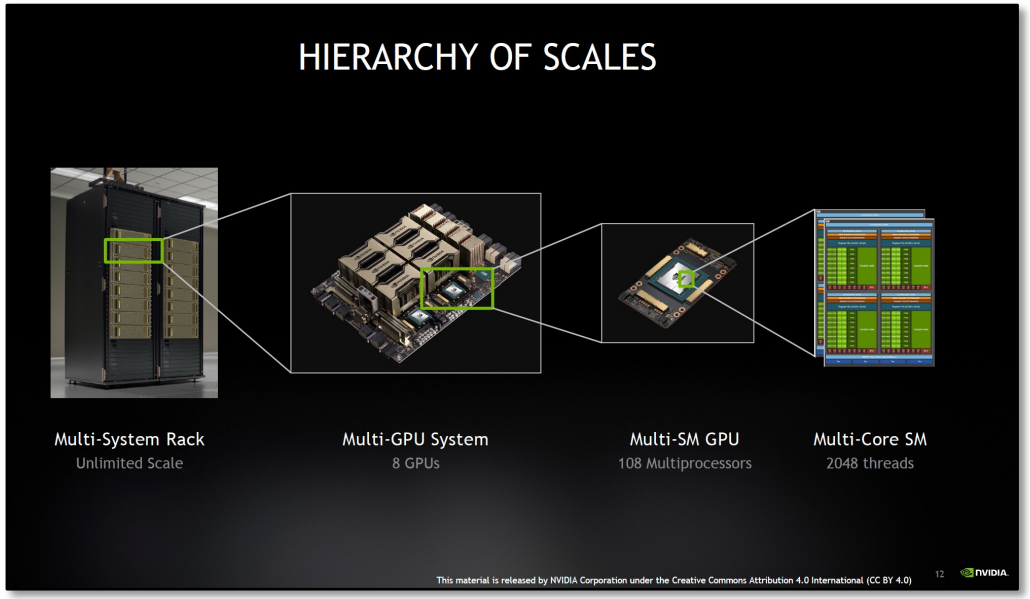
IMPACT: Investigating other architectures that may provide improvements over HECC's currently available hardware provides valuable inputs for future HECC procurement decision.

NEC Vector Systems in a rack at the NASA Advanced Supercomputing facility. *Don Story, NASA/Ames*

GPU Bootcamps Held for AI/ML and HPC Applications

- Two 8-hour virtual bootcamps, aimed at orienting individuals with no prior Graphics Processing Unit (GPU) experience, were hosted by staff in the NASA Advanced Supercomputing Division. The sessions served as training events for the upcoming NASA GPU Hackathon in September.
- One session on June 28–29 focused on background material for Artificial Intelligence/Machine Learning technologies; the other on July 6–7 covered traditional HPC-centric approaches.
- The events were a collaboration between Nvidia and HECC's Data Science and Application Performance and Productivity teams.
  - Nvidia provided Singularity containers and Jupyter notebooks to allow hands-on interactive experience for participants when working on example codes. The HECC team thoroughly tested all containers prior to the event.
  - HECC allocated 15 V100 GPU nodes to support the event.
  - The HECC teams ran a pre-bootcamp session to familiarize users with singularity containers and Jupyter notebooks in the HECC environment.
  - Zoom and Slack were used for virtual collaboration and communication.
  - Several highly qualified instructors and mentors from Nvidia and HECC assisted participants in solving challenging example problems.
  - About 20 participants attended the events.

IMPACT: Training provided by expert teams during the GPU bootcamps prepared users for an upcoming GPU Hackathon by introducing them to the concept and approach of accelerated computing on GPU nodes at the NASA Advanced Supercomputing facility.

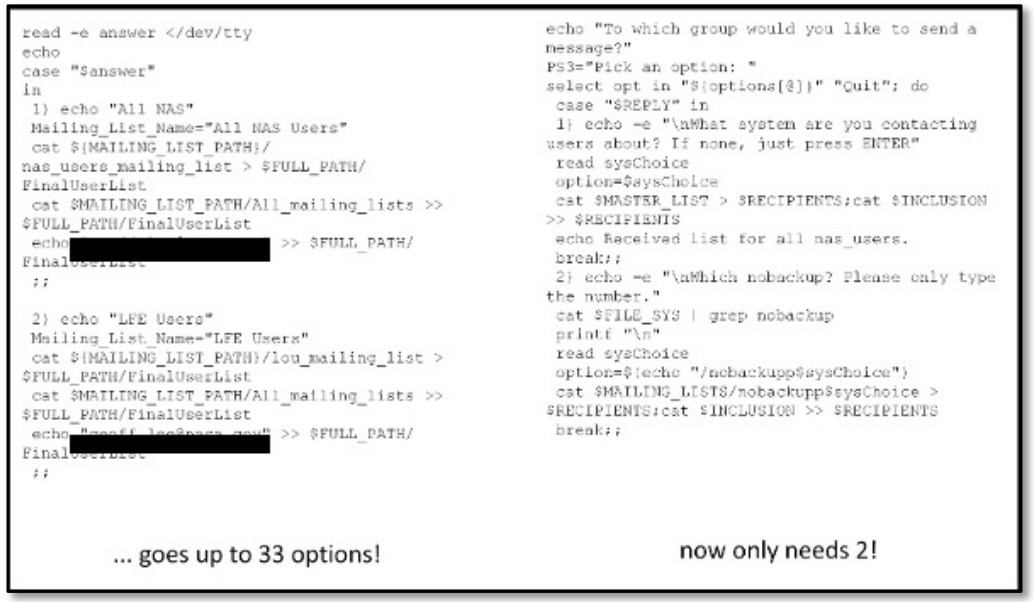


Graphic depicting the hierarchy of parallelism available in a cluster of GPU nodes. *Image courtesy of Nvidia*

Overhauling the Control Room's Mailer: nasops_mailer

- The nasops_mailer is a set of scripts used by the NAS Control Room to automate the management of email lists of HECC supercomputing system users.
- The original nasops_mailer was prone to errors and difficult to use and maintain due to configuration issues and lack of documentation. Control Room analysts (CRAs) reviewed the original version and implemented the following changes:
  - Modularized the original script (which had all logic and configuration in one file) to reside in multiple files in order to improve understandability and ease of maintenance.
  - Changed access permissions required of CRAs to run the script to email users: previously, root access was required; now, only Control Room's Project GID is needed.
  - Relocated the install location to allow CRAs to run the nasops_mailer from either Pleiades front-end or Lou front-end hosts.
  - Updated the mailing list creation process to restrict new lists to active users, and simplified the process by which lists based on subsets of users are generated (for example, /nobackupp17 users)
  - Created a backup process for mailing lists and a custom log rotation functionality to restrict the volume of backed-up mailing lists.
- These upgrades were documented and have simplified distributing messages to users, standardized the messages, and made the script maintainable.

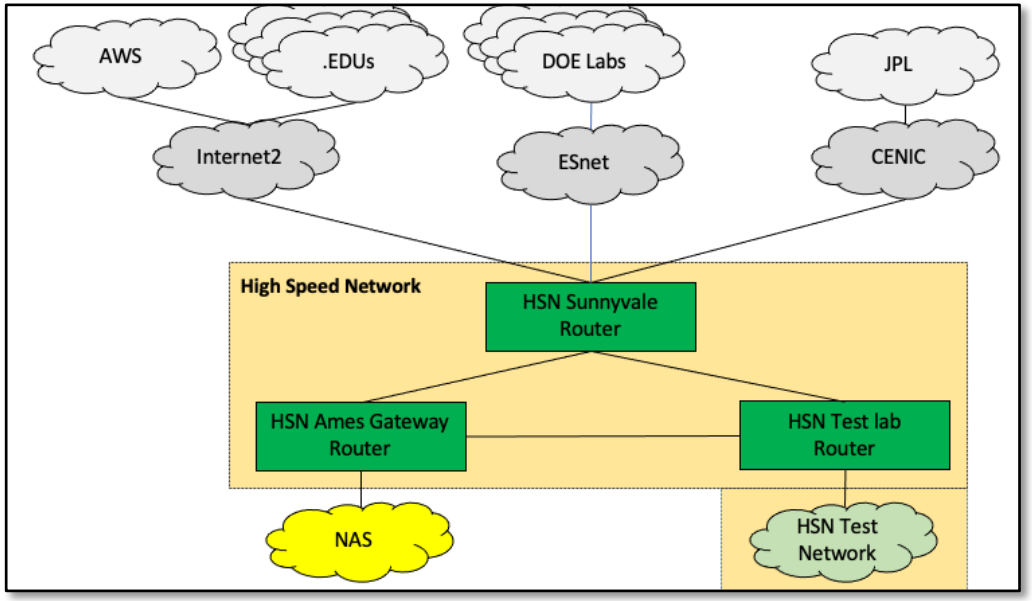
IMPACT: Revamping and documenting the nasops_mailer simplified its use and maintenance for the Control Room staff and increased the reliability of emails being sent to groups of users.



HECC Upgrades High Speed Network Infrastructure

- The HECC Networks team completed upgrades to network hardware in the High Speed Network (HSN) infrastructure.
- The enhancements provide faster network throughput—increased from 10 gigabits per second to 100 gigabits per second—and increase the capacity for users to transfer data to and from the HECC Enclave.
  - Positions the HSN to increase network bandwidth with peering partners such as Internet2 and CENIC.
  - Provides improved system performance:
    - Switch backplane speed up to 3.2 terabytes per second.
    - Increased system capabilities (Faster CPU, increased memory, increased ability to store IPv4 / IPv6 routes).
- In addition, the upgrade positions the HSN to establish dedicated high-speed network connectivity to cloud providers/partners such as Amazon Web Services and Azure, and improves the HSN security posture:
  - The HSN infrastructure now incorporates new hardware and the latest vendor recommended firmware.
  - The old network infrastructure (hardware and firmware) was end-of-life.

IMPACT: These major upgrades to HECC's high-speed network infrastructure increase network capacity and capability in order to enhance the user experience for scientists and engineers transferring important data for NASA projects and missions.

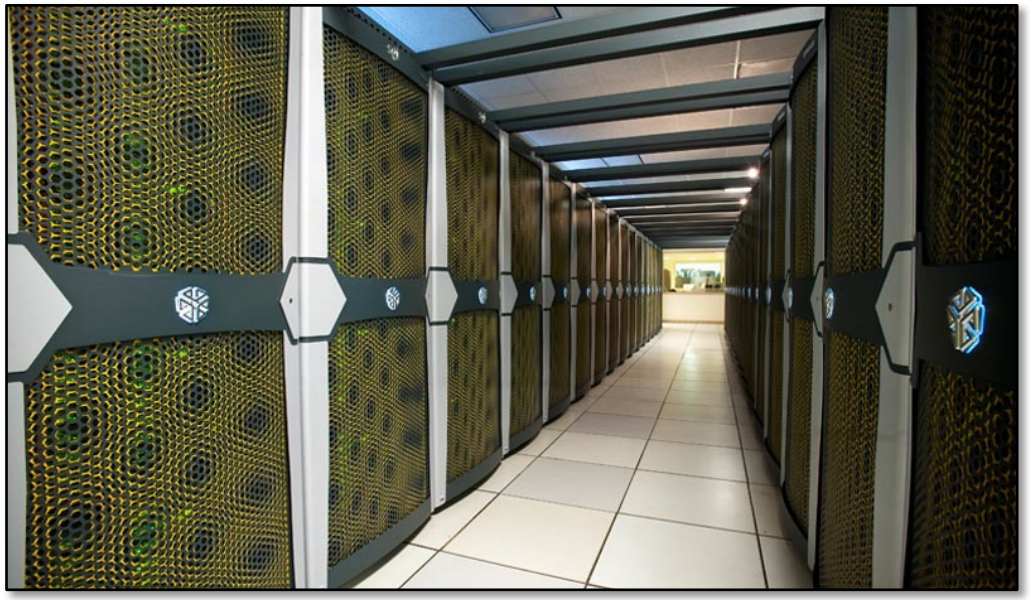


Overview of HSN connectivity. The three HSN routers were replaced during this activity. *HECC Networks Group*

HECC Teams Excess Computer Racks, Update Processes

- The HECC Systems, Property, and Facilities teams worked together to identify and excess 49 decommissioned computer racks, and prepared the equipment for removal and disposal by the Ames Logistics Group.
  - 45 Westmere racks were excessed.
  - 4 Endeavour racks were excessed.
- Preparation for excessing the racks included:
  - Identifying and marking the racks.
  - Removing 98 hard drives from the racks.
  - Removing cabling and power whips.
  - Unfastening the wheels and lowering the leveler feet.
  - Coordinating with movers to remove the racks from Building N258.
- During completion of this excess, the teams identified gaps in the current processes and are creating new forms and checklists to standardize the decommissioning and excessing of large equipment in an efficient manner.
- Removing the 49 racks allowed HECC to reclaim more than 360 square feet of computer floor space (equivalent to three rows of equipment) for future expansion.

IMPACT: By excessing outdated computer equipment, HECC frees physical space and electrical, cooling, and network resources for new equipment



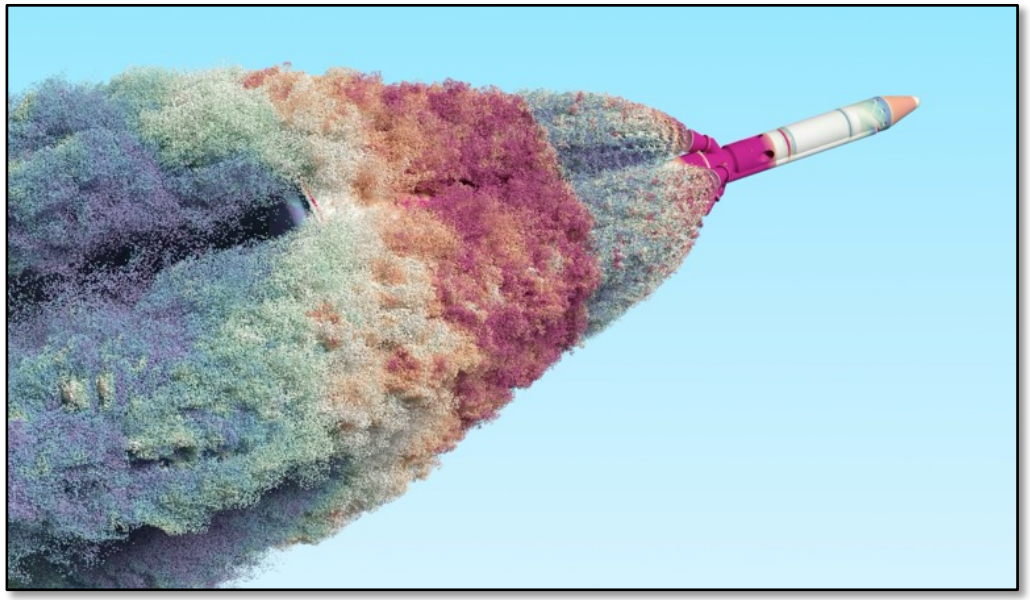
Two rows of Pleiades Westmere-based racks. *NASA Ames*

Predicting Orion Ascent Abort Acoustics for Crew Safety*

- Computational fluid dynamics (CFD) experts in the NASA Advanced Supercomputing Division ran turbulence-resolving simulations of the Orion Launch Abort System (LAS) using their Launch Ascent and Vehicle Aerodynamics (LAVA) framework on the Electra and Aitken supercomputers.
  - To propel the crew module away to safety in the event of an emergency during launch, the LAS uses a solid rocket motor that produces four large high-speed exhaust plumes that flow along the sides of Orion, generating extremely strong acoustic vibrations. Abort could be triggered at any time during launch—on the pad or during ascent.
  - The team simulated eight different launch abort scenarios, investigating the effects of modeling the attitude control motors for abort at supersonic speed—and the impact of the altitude and velocity when abort is triggered—on the strength and spatial distribution of the acoustic vibrations on the vehicle's surface.
  - The researchers also significantly improved LAVA's CFD acoustic prediction capability by refactoring the algorithms and data structures to increase parallel efficiency and reduce turnaround time.
- The LAVA team has collaborated with the Orion Loads and Dynamics team since 2017 to help characterize the vibrations imparted onto the vehicle by the LAS motor plumes.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: These CFD predictions help reduce uncertainty for abort scenarios that are difficult or too expensive to test—like the high-altitude, near-hypersonic abort—further helping NASA reduce risk and ensure the safety of astronauts during a potential launch abort.



Visualization of a simulated ascent of the AA-2 launch abort vehicle. Passive particles highlight the abort motor's high-speed turbulent exhaust plumes generating strong vibrations on the vehicle; particles and the vehicle surface are colored by gauge pressure (blue is low, red is high). *Francois Cadieux, Timothy Sandstrom, NASA/Ames*

Papers

- "**Improving the Performance of a Compressible RANS Solver for Low and High Mach Numbers Flows**," S. Seraj, et al., presented at the 11th International Conference on Computational Fluid Dynamics (ICCFD11), Maui, HI, July 11-15, 2022. *
  https://www.researchgate.net/publication/361880059_Improving_the_Performance_of_a_Compressible_RANS_Solver_for_Low_and_High_Mach_Number_Flows
- "**Shock Breakout in Three-Dimensional Red Supergiant Envelopes**," J. Goldberg, Y.-F. Jiang, L. Bildsten, The Astrophysical Journal, vol. 933, no. 2, July 12, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ac75e3/meta
- "**Ram Pressure Stripping of the Multiphase ISM: A Detailed View from TIGRESS Simulations**," W. Choi, C.-G. Kim, A. Chung, arXiv:2207.05263 [astro-ph.GA] July 12, 2022. *
  https://arxiv.org/abs/2207.05263
- "**Suppressing Quantum Errors by Scaling a Surface Code Logical Qubit**," R. Acharya, et al., arXiv:2207.06431 [quant-ph], July 13, 2022. *
  https://arxiv.org/abs/2207.06431
- "**High-Contrast Imaging of HD 29992 and HD 196385 with GPI**," L. Garcia, R. Petrucci, E. Jofre, M. Gomez, arXiv:2207.07435 [astro-ph.SR], July 15, 2022. *
  https://arxiv.org/abs/2207.07435
- "**Asteroseismology Reveals the Near-Core Magnetic Field Strength in the Early-B Star HD 43317**," D. Bowman, D. Lecoanet, T. Van Reeth, arXiv:2207.08526 [astro-ph.SR], July 18, 2022. *
  https://arxiv.org/abs/2207.08526

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Stellar Energetic Particle Transport in the Turbulent and CME-disrupted Stellar Wind of AU~Microscopii**," F. Fraschetti, J. Alvarado-Gomez, J. Drake, O. Cohen, C. Garraffo," arXiv:2207.08952 [astro-ph.SR], July 18, 2022. *
https://arxiv.org/abs/2207.08952
- "**A Truncated Davidson Method for the Efficient 'Chemically Accurate' Calculation of Full Configuration Interaction Wavefunctions without any Large Matrix Diagonalization**," S. Cotton, arXiv:2207.12587 [physics.chem-ph], July 26, 2022. *
https://arxiv.org/abs/2207.12587
- "**Methane Emission From Global Lakes: New Spatiotemporal Data and Observation-Driven Modeling of Methane Dynamics Indicates Lower Eminissions**," M. Johnson, E. Matthews, J. Du, V. Genovese, D. Bastviken, Journal of Geophysical Research: Biogeosciences, vol. 127, issue 7, July 27, 2022. *
https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2022JG006793
- "**The Interplay Between Twinning and Cation Inversion in $MgAl_2O_4$-spinel: Implications for a Nebular Thermochronometer**," V. Manga, K. Muralidharan, T. Zega, American Mineralogist, published online July 27, 2022. *
https://www.degruyter.com/document/doi/10.2138/am-2021-7874/html
- "**Atmosphere of the Mini-Neptune Transiting the Bright M Dwarf GJ3090 Can be Characterized**," J. Almenara, et al., arXiv:2207.14121 [astro-ph.EP], July 28, 2022. *
https://arxiv.org/abs/2207.14121
- "**The HD 93963 A Transiting System: A 1.04d Super-Earth and a 3.65 d Sub-Neptune Discovered by TESS and CHEOPS**," L. Serrano, et al., arXiv:2207.13920 [astro-ph.EP], July 28, 2022. *
https://arxiv.org/abs/2207.13920

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Papers (cont.)

- "**Packed Media Radiative-Transfer Modeling with Gaussian Particles: Application to Spectra of Icy Regolith of Saturnian Satellites**," G. Ito, L. Kolokolova, D. Petrov, K. Pitman, Journal of Quantitative Spectroscopy and Radiative Transfer, published online July 28, 2022. *
  https://www.sciencedirect.com/science/article/abs/pii/S0022407322002552
- "**Solar Observatories**," P. Bond, Solar Surveyors (Springer), published online July 30, 2022. *
  https://link.springer.com/chapter/10.1007/978-3-030-98788-6_5

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Presentations

- **11th International Conference on Computational Fluid Dynamics (ICCFD11)**, Maui, HI, July 11–15, 2022. (abstracts)
  - "**Algorithmic Improvements to a High-Order Space Marching Method for Sonic Boom Propagation**," J. Housman, et al. *https://www.iccfd.org/iccfd11/assets/pdf/abstracts/ICCFD11_Abstract-1205.pdf*
  - "**Validation of Actuator Disk, Actuator Line and Sliding Mesh Methods within the LAVA Solver**," G.-D. Stich, et al. *https://www.iccfd.org/iccfd11/assets/pdf/abstracts/ICCFD11_Abstract-0903.pdf*
  - "**Distribution of SLS Integrated Load Uncertainty to Surface Pressures and Sectional Loads**," D. Dalle, et al. *https://www.iccfd.org/iccfd11/assets/pdf/abstracts/ICCFD11_Abstract-3303.pdf*
  - "**Flow Field Reconstruction for Inhomogeneous Turbulence using Data and Physics Driven Models**," A. Ghate, et al. *https://www.iccfd.org/iccfd11/assets/pdf/abstracts/ICCFD11_Abstract-3105.pdf*
  - "**Recent Development of High Order Entropy Split Methods for Compressible Gas Dynamics and MHD**," H. Yee, et al. *https://www.iccfd.org/iccfd11/assets/pdf/abstracts/ICCFD11_Abstract-3503.pdf*

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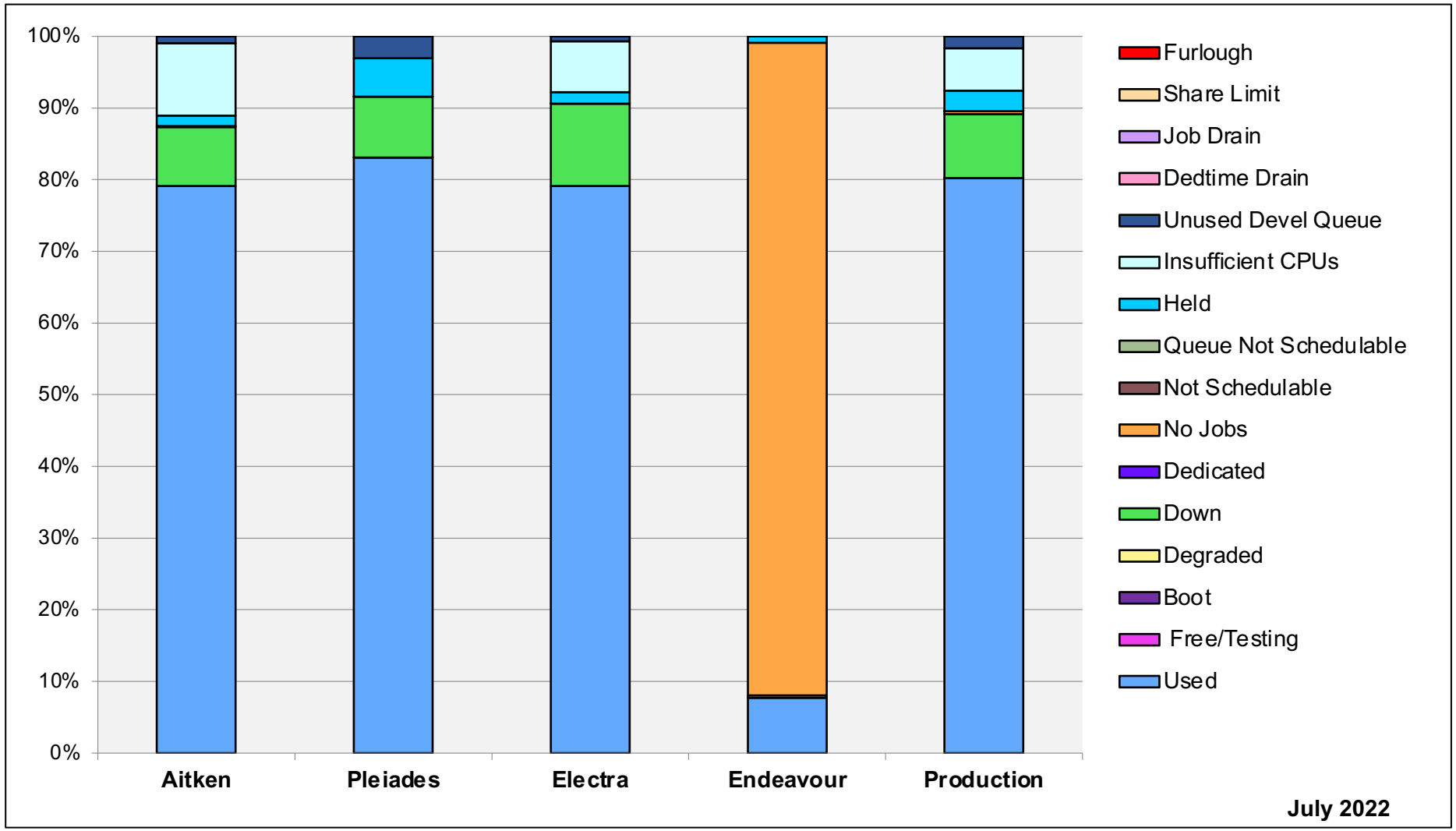
News and Events

- **Aitken Leaps Over Pleiades to Become NASA's Most Powerful Supercomputer**, *NASA Advanced Supercomputing Division,* July 13, 2022—With its latest expansion, the Aitken supercomputer became NASA's most powerful high-performance computing (HPC) system—surpassing the agency's longtime HPC workhorse, Pleiades, which had held the title for the past 14 years.
  https://www.nas.nasa.gov/pubs/stories/2022/feature_Aitken_expansion_2Q2022.html
  - **Aitken Becomes NASA's Most Powerful Supercomputer**, *HPCwire*, July 19, 2022.
    https://www.hpcwire.com/off-the-wire/aitken-becomes-nasas-most-powerful-supercomputer/
  - **The Latest NASA Supercomputer is a Bit of a DIY Masterpiece**, *TechRadar*, July 20, 2022.
    https://www.techradar.com/news/the-latest-nasa-supercomputer-is-a-diy-masterpiece
  - **NASA Pulls Together Pieces for Its Most Powerful Supercomputer Yet**, *The Register,* July 20, 2022.
    https://www.theregister.com/2022/07/20/nasa_pulls_together_pieces_for/

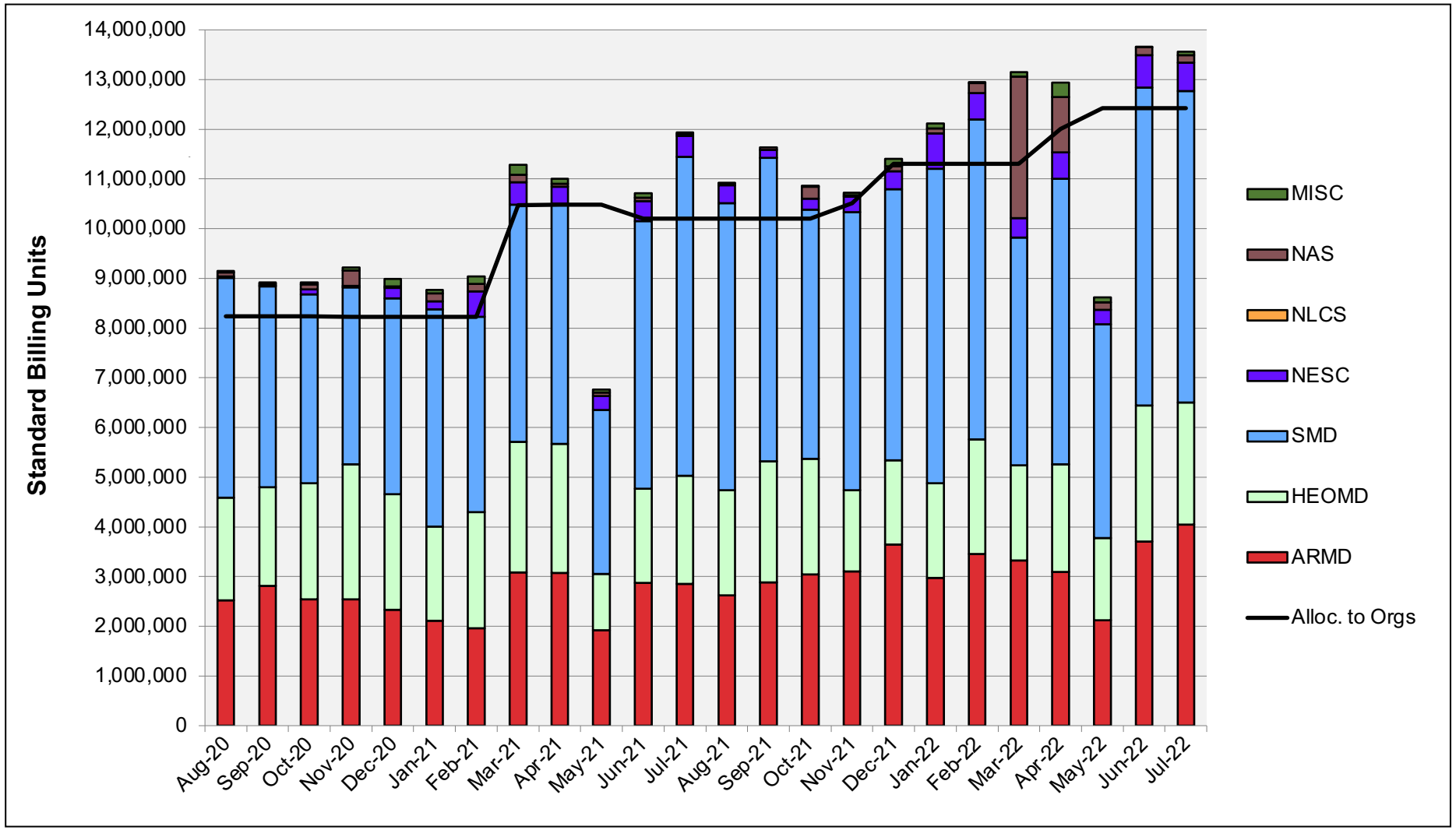
News and Events: Social Media

- **Coverage of NAS Stories**
  - FY21 Annual Report Available:
    - NAS: Twitter 5 retweets.
  - Aiken Expansion Story:
    - NAS: Twitter 4 retweets, 14 favorites.
    - NASA Supercomputing: Twitter 3 retweets, 12 likes; Facebook 867 users reached, 292 views, 54 reactions/shares.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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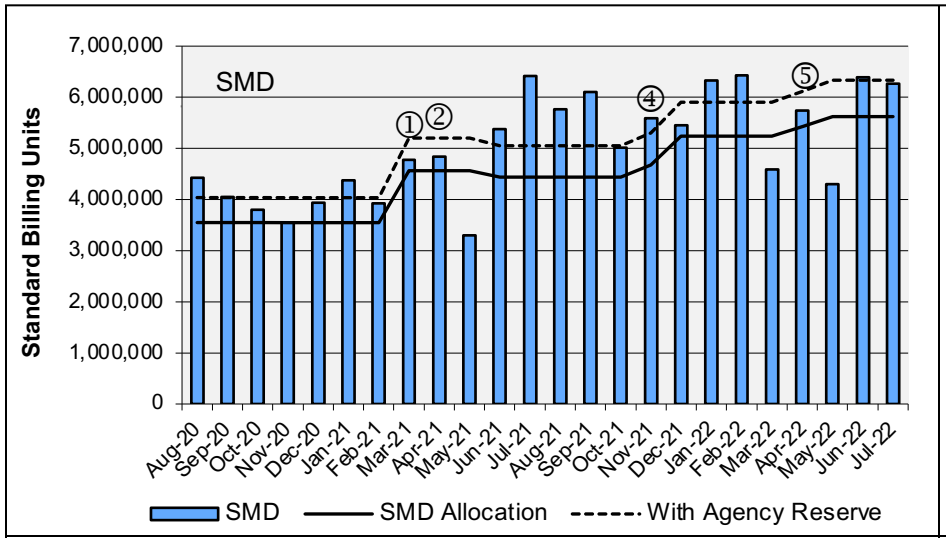
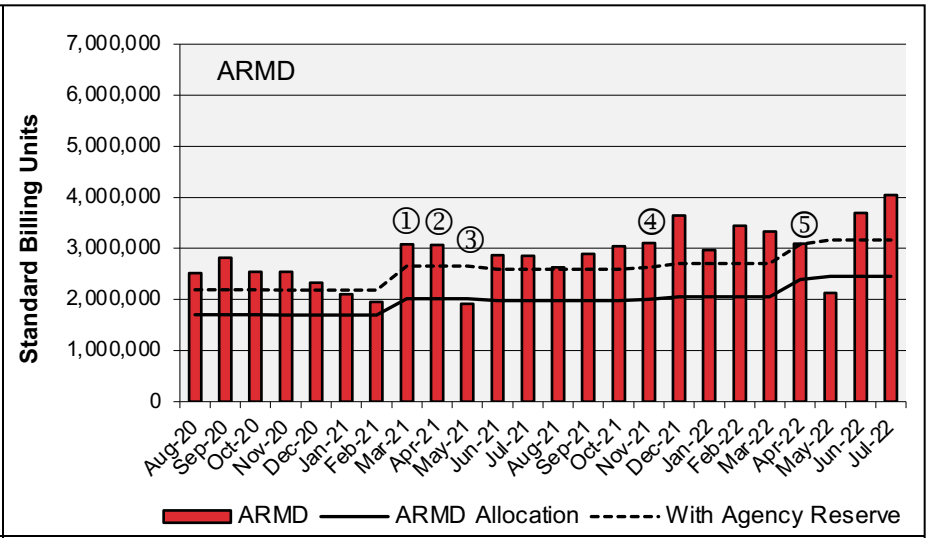
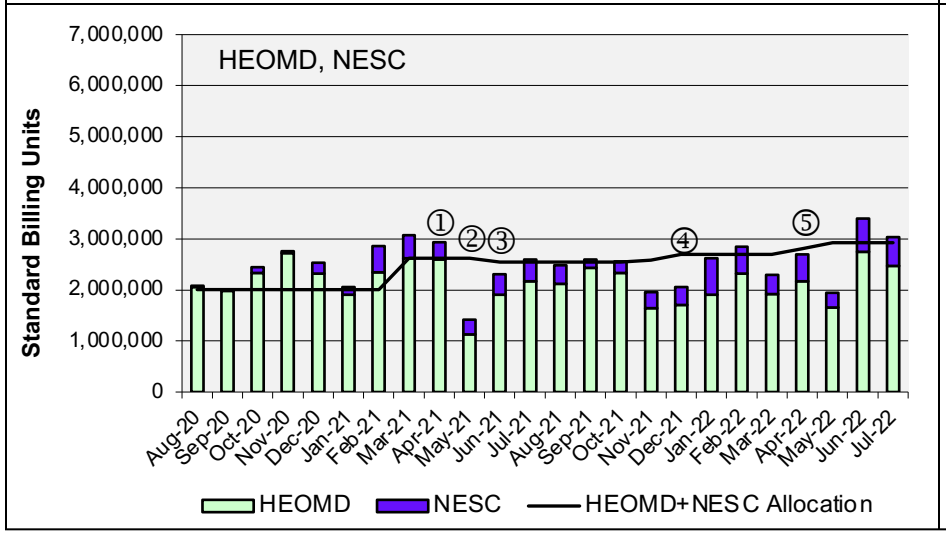






① 8 Rome Apollo racks introduced into Aitken

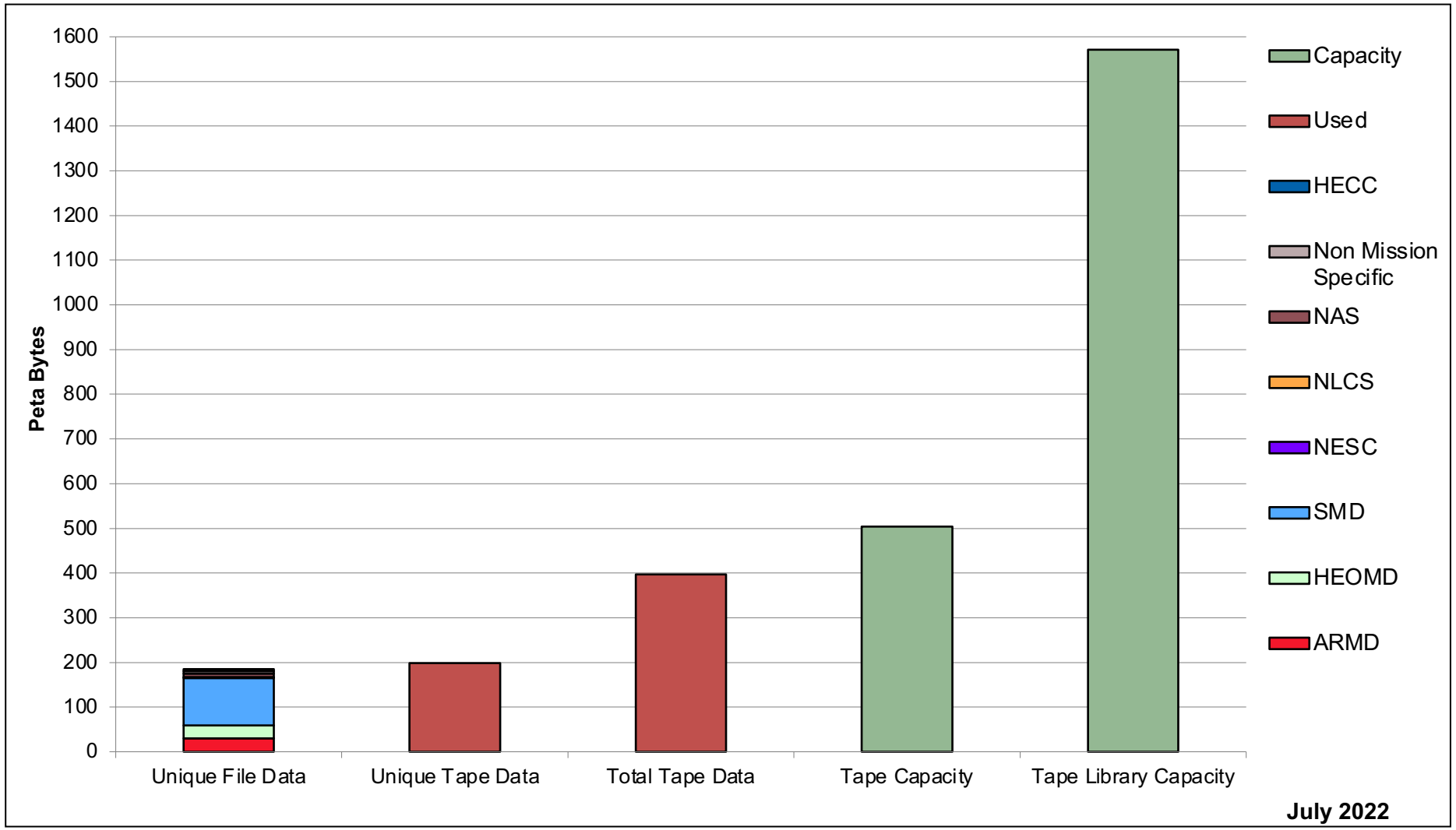
② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

⑤ 4 Rome Apollo Racks added to Aitken

Tape Archive Status



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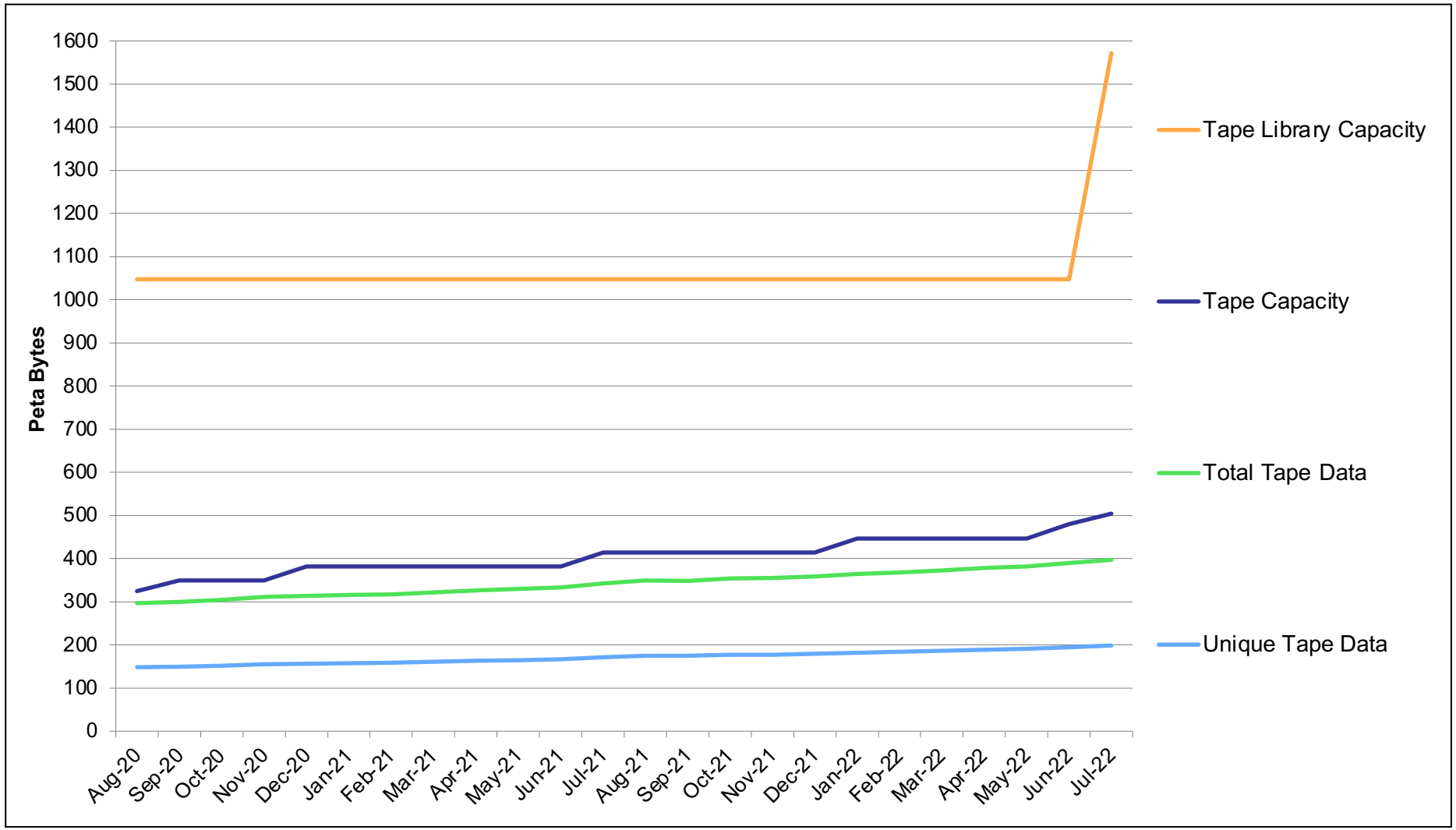
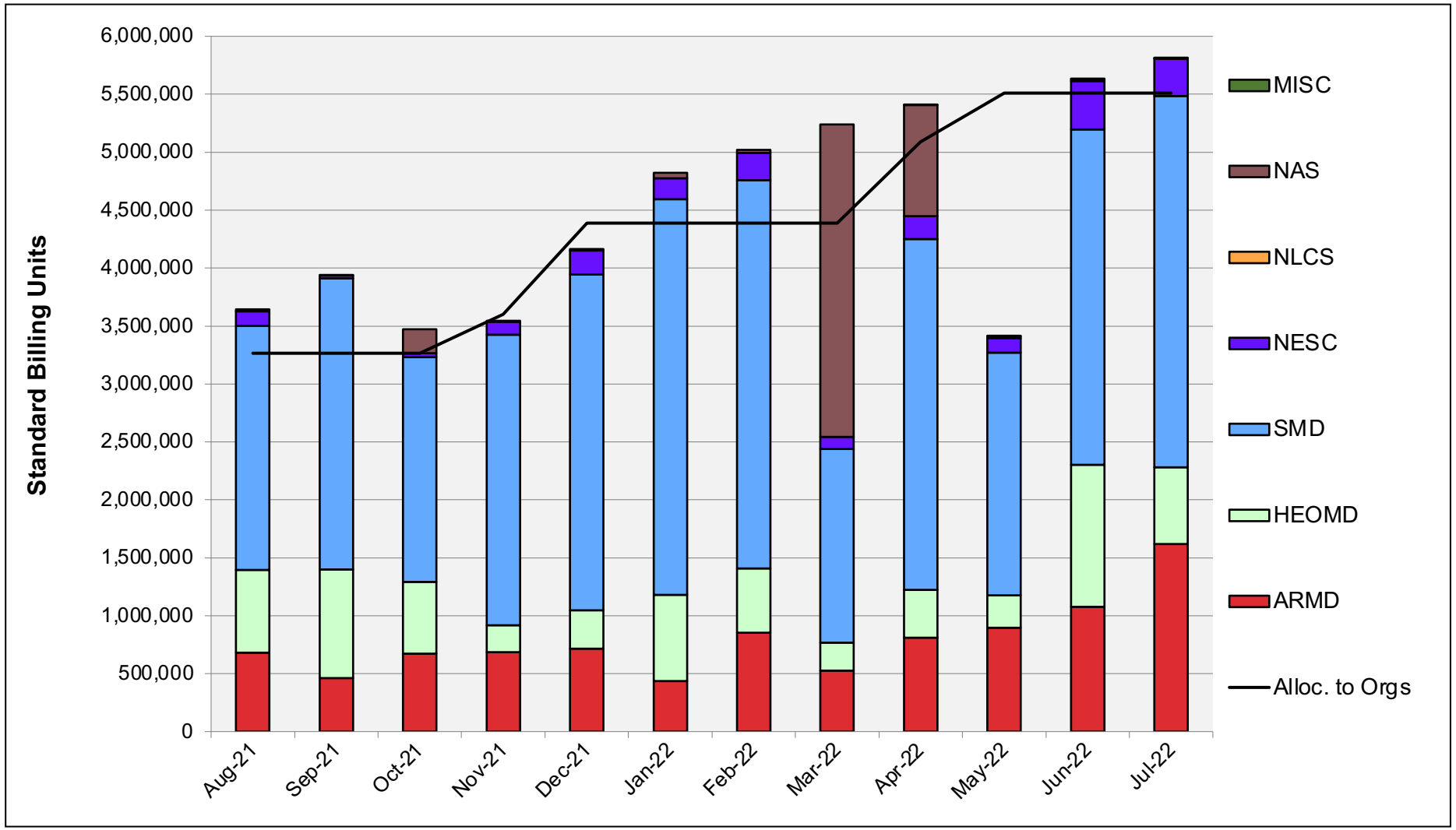
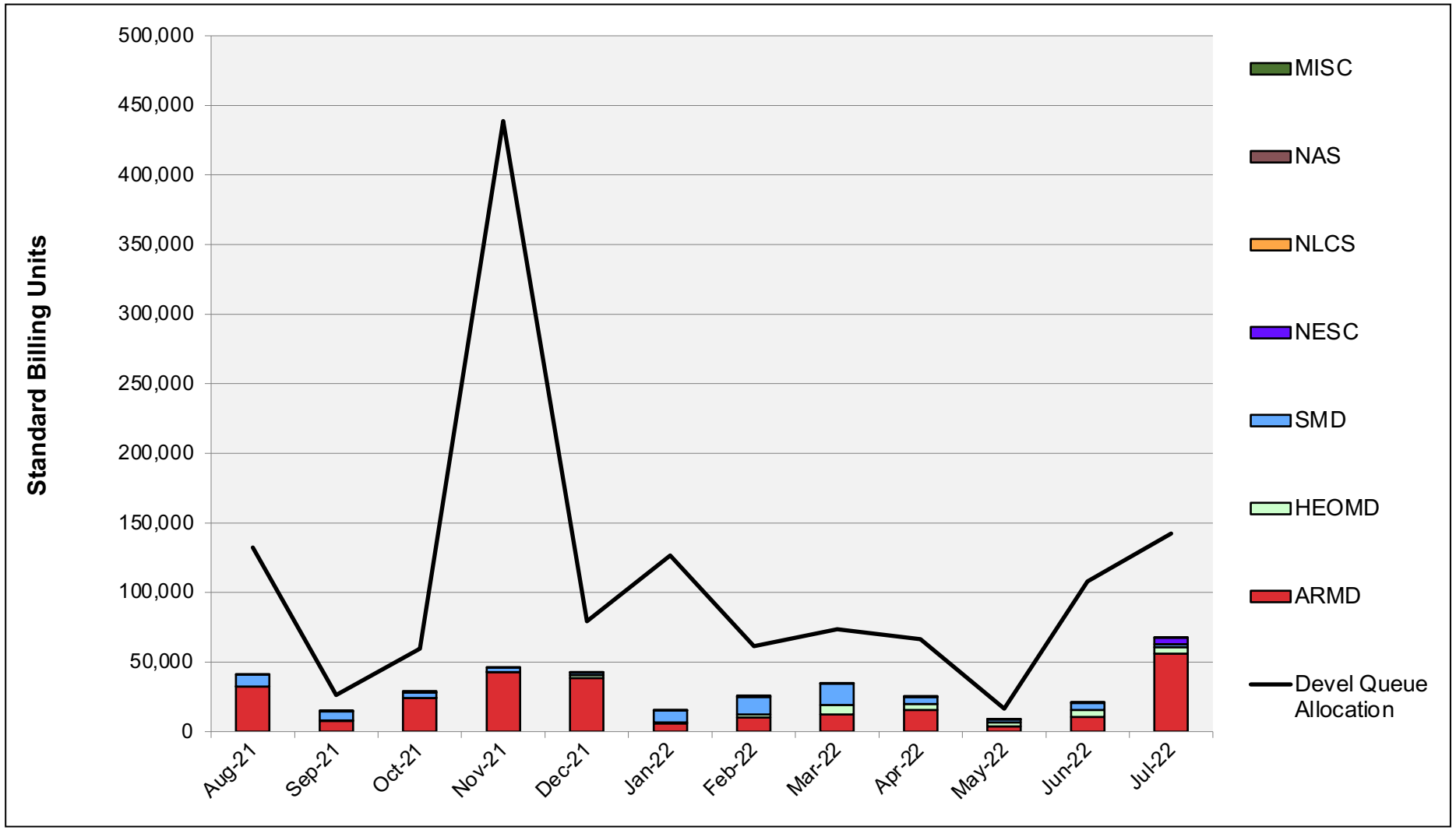


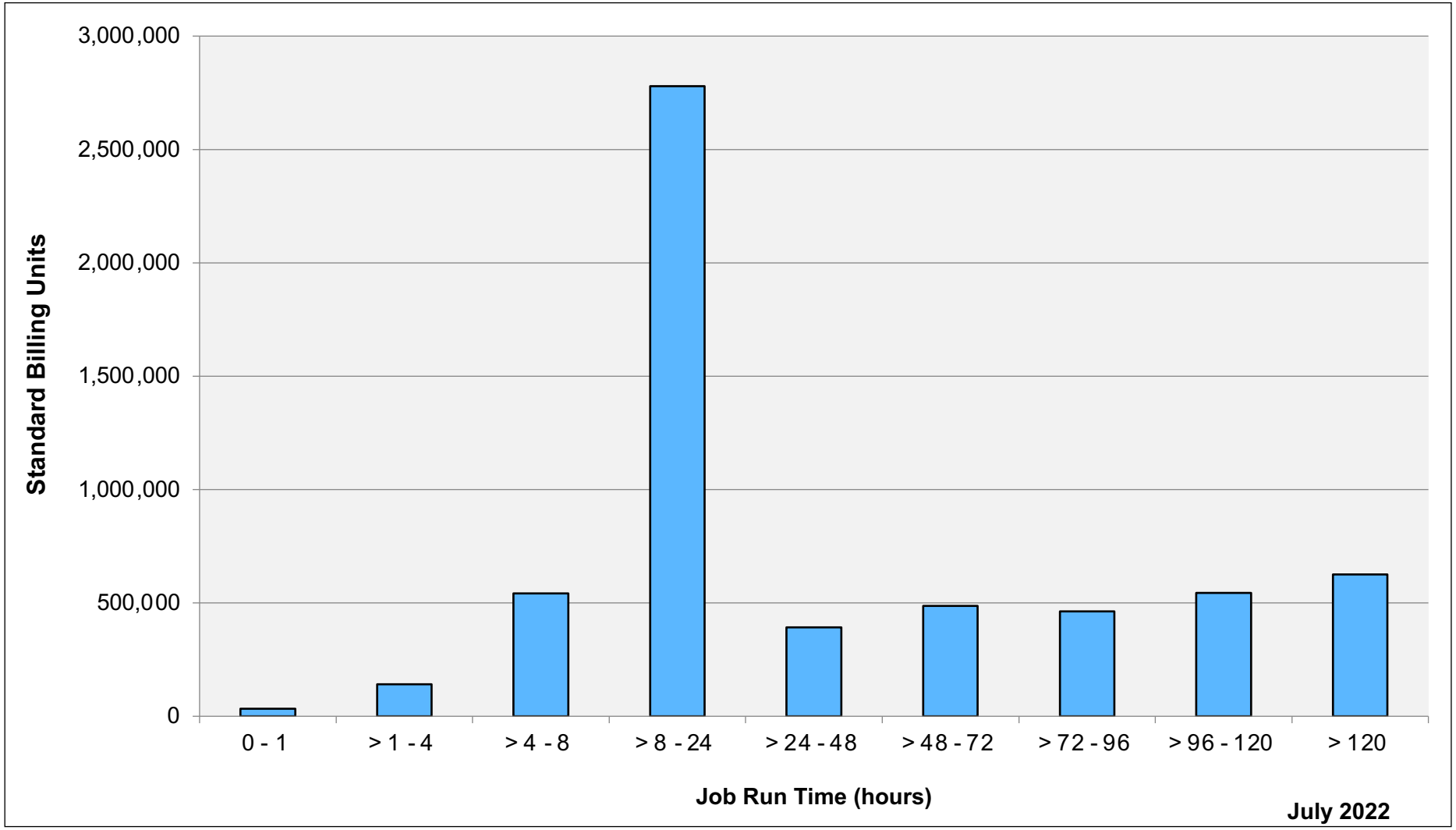
Aitken: SBUs Reported, Normalized to 30-Day Month



Aitken: Devel Queue Utilization



Aitken: Monthly Utilization by Job Length



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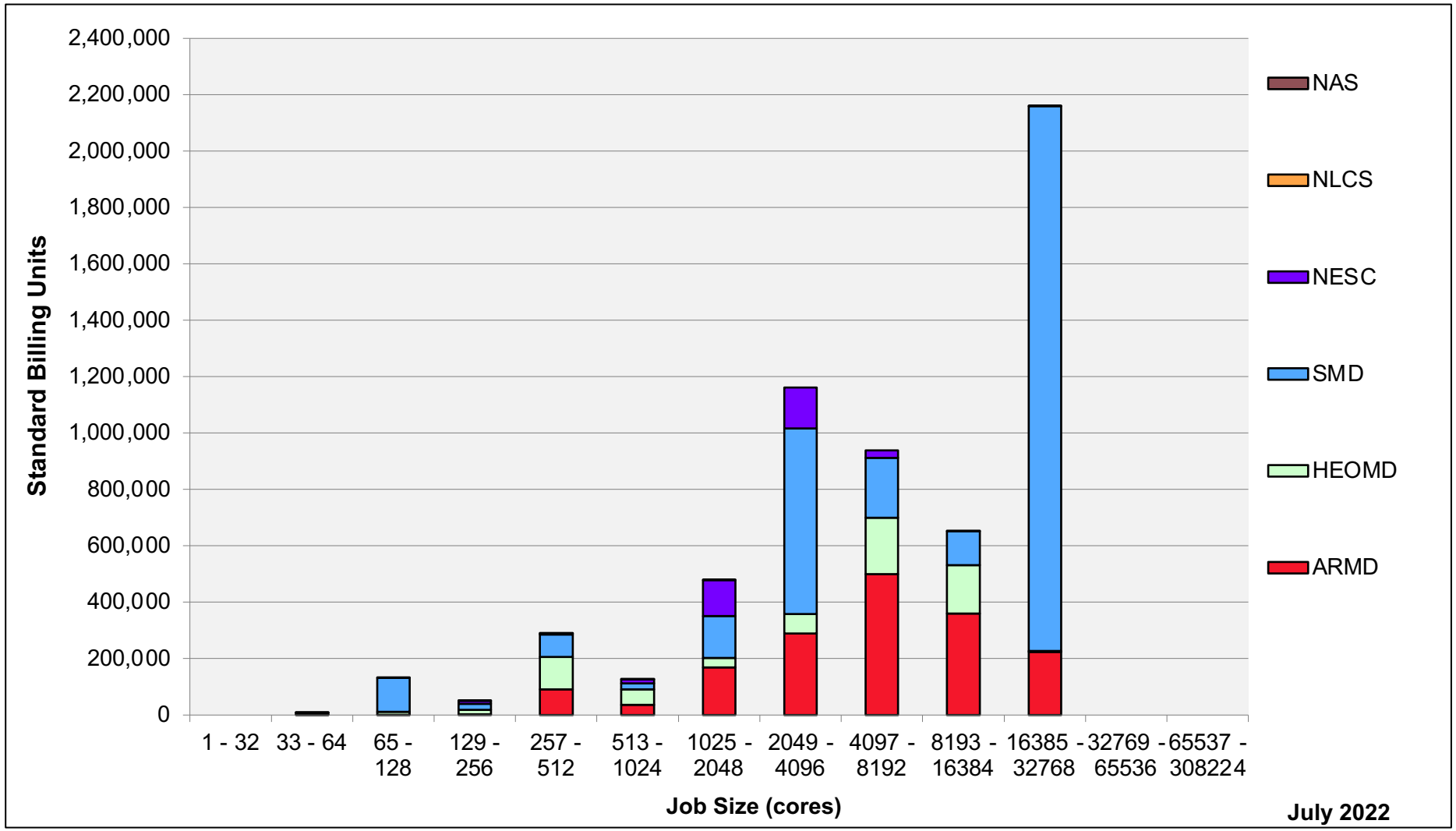
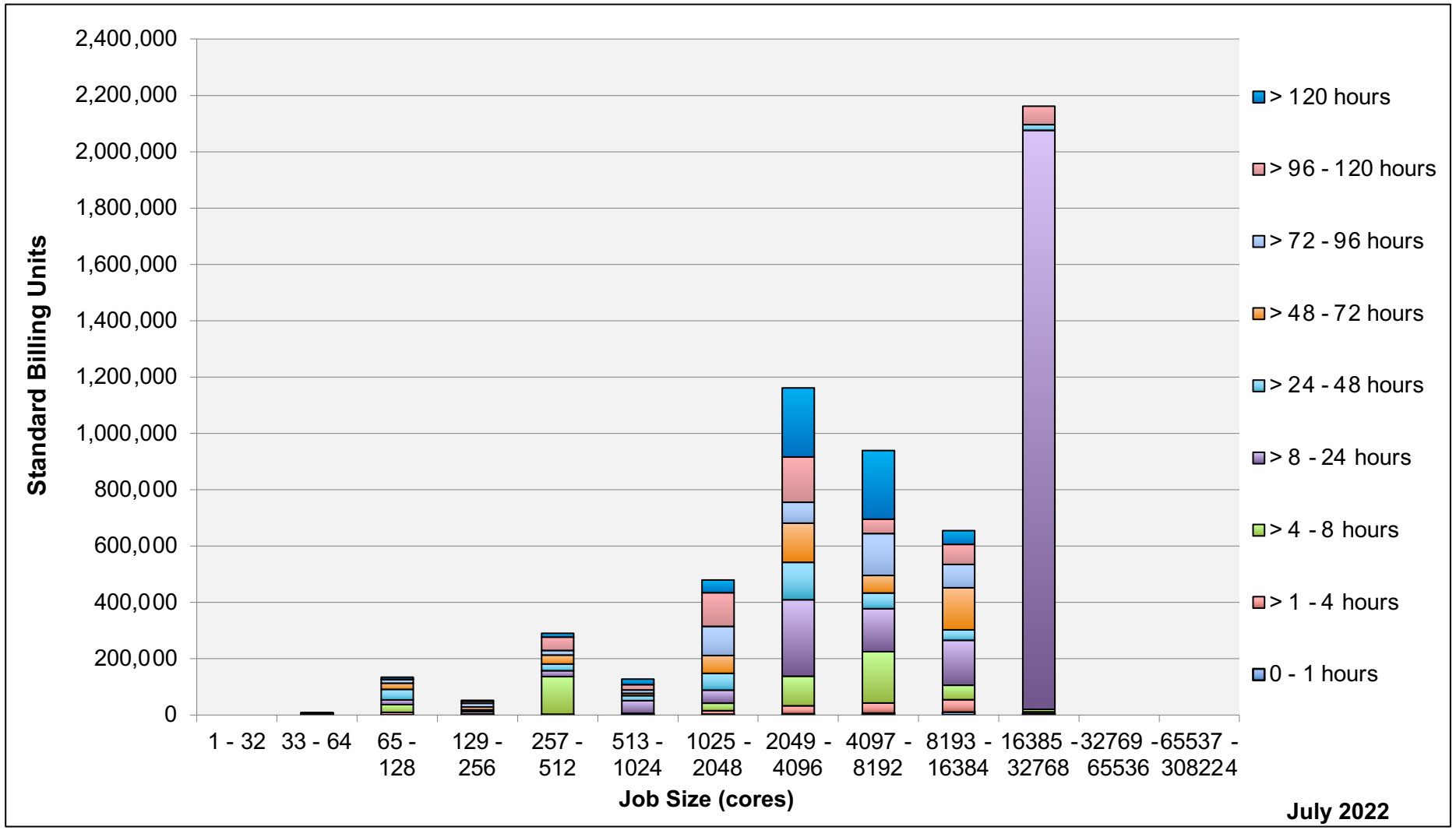
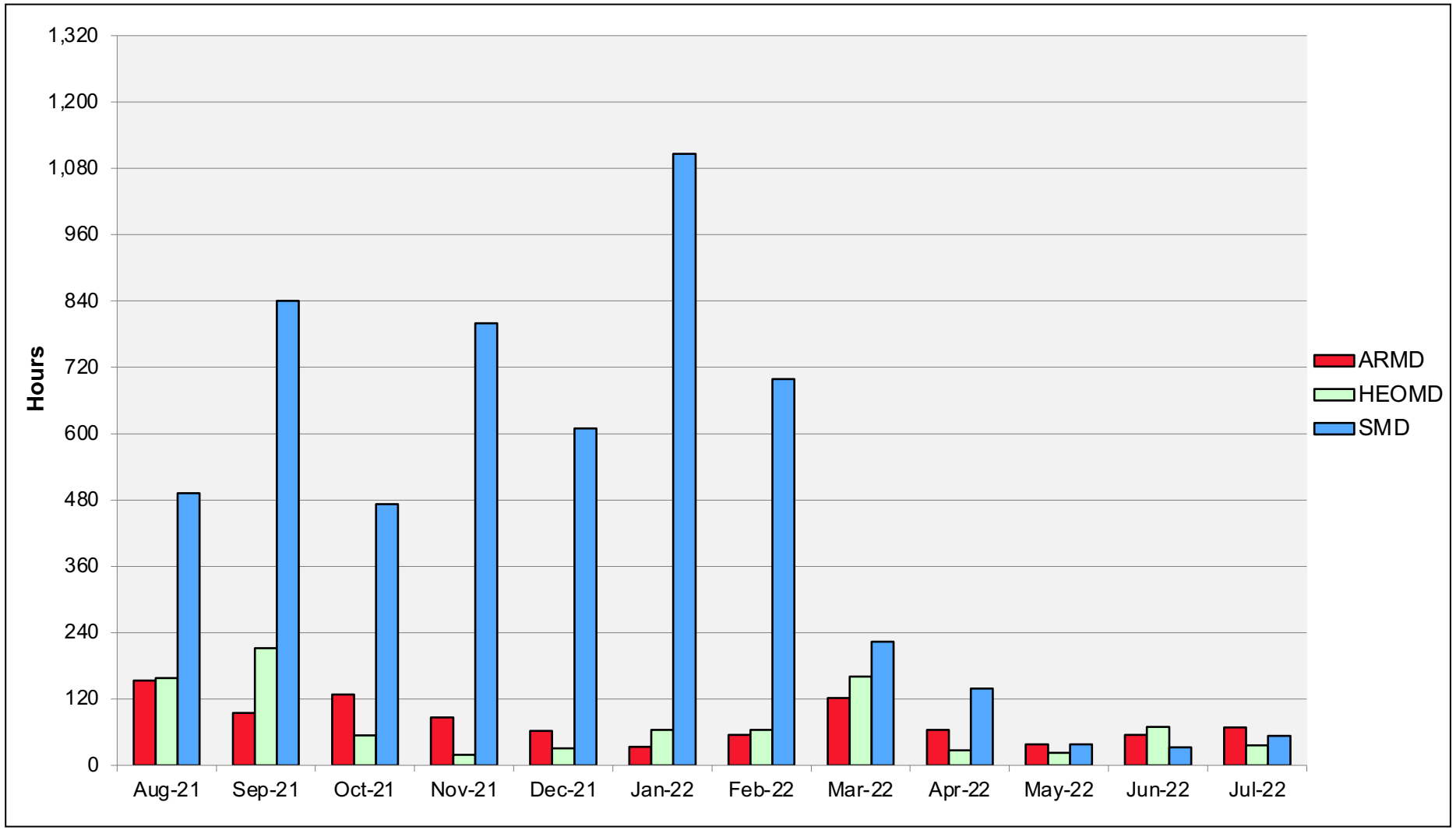


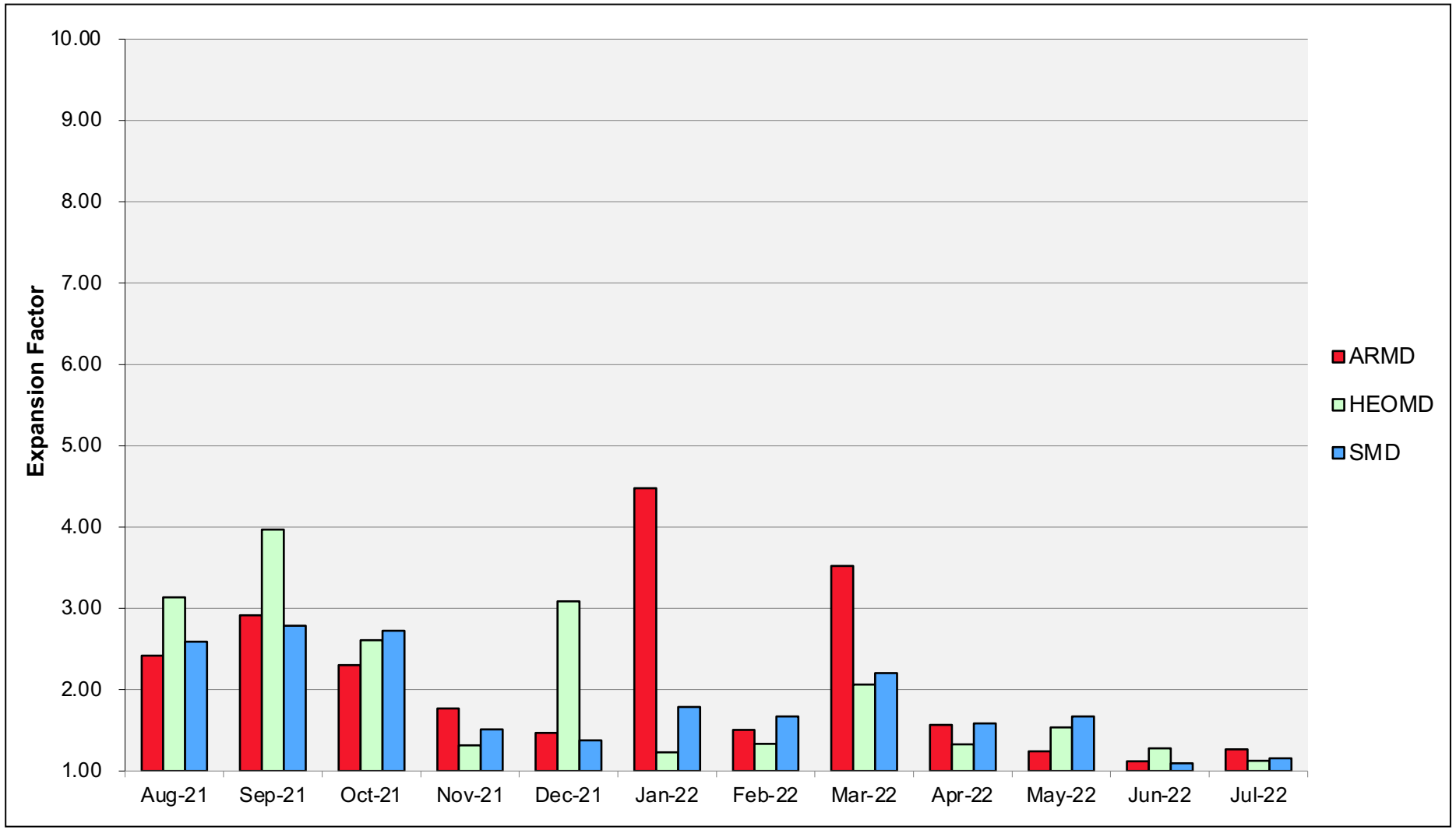
Aitken: Monthly Utilization by Size and Length



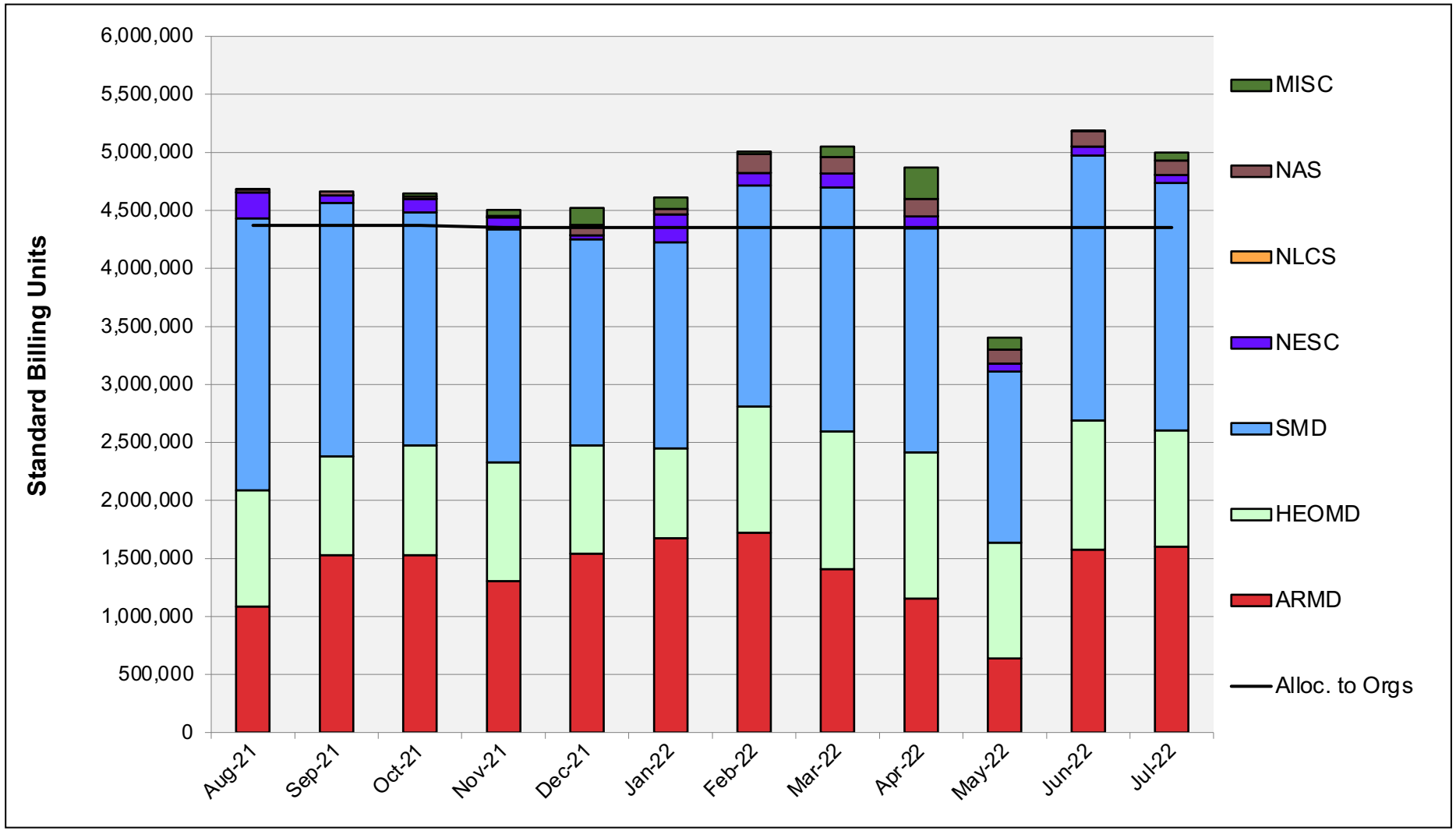
Aitken: Average Time to Clear All Jobs



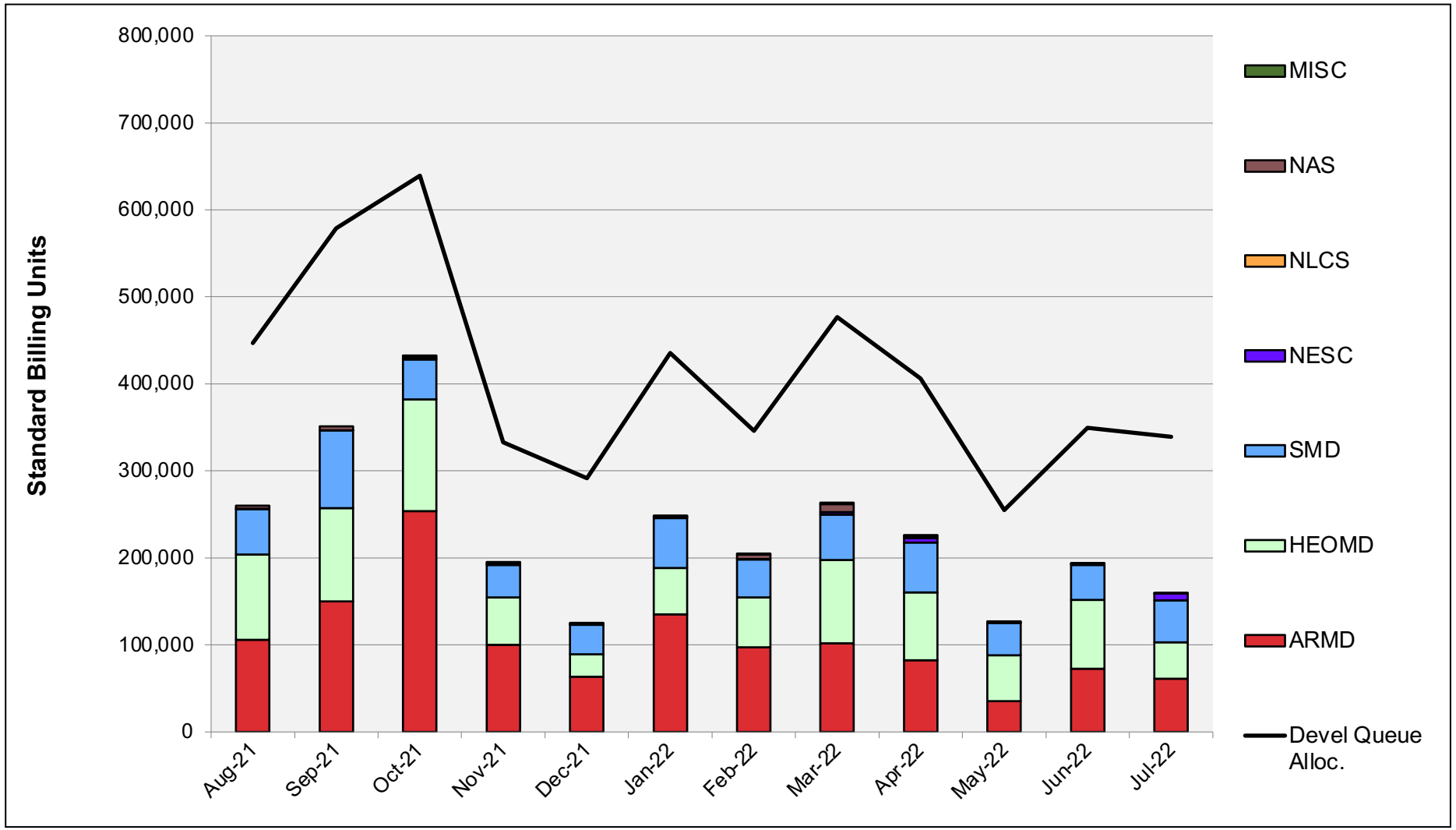
Aitken: Average Expansion Factor



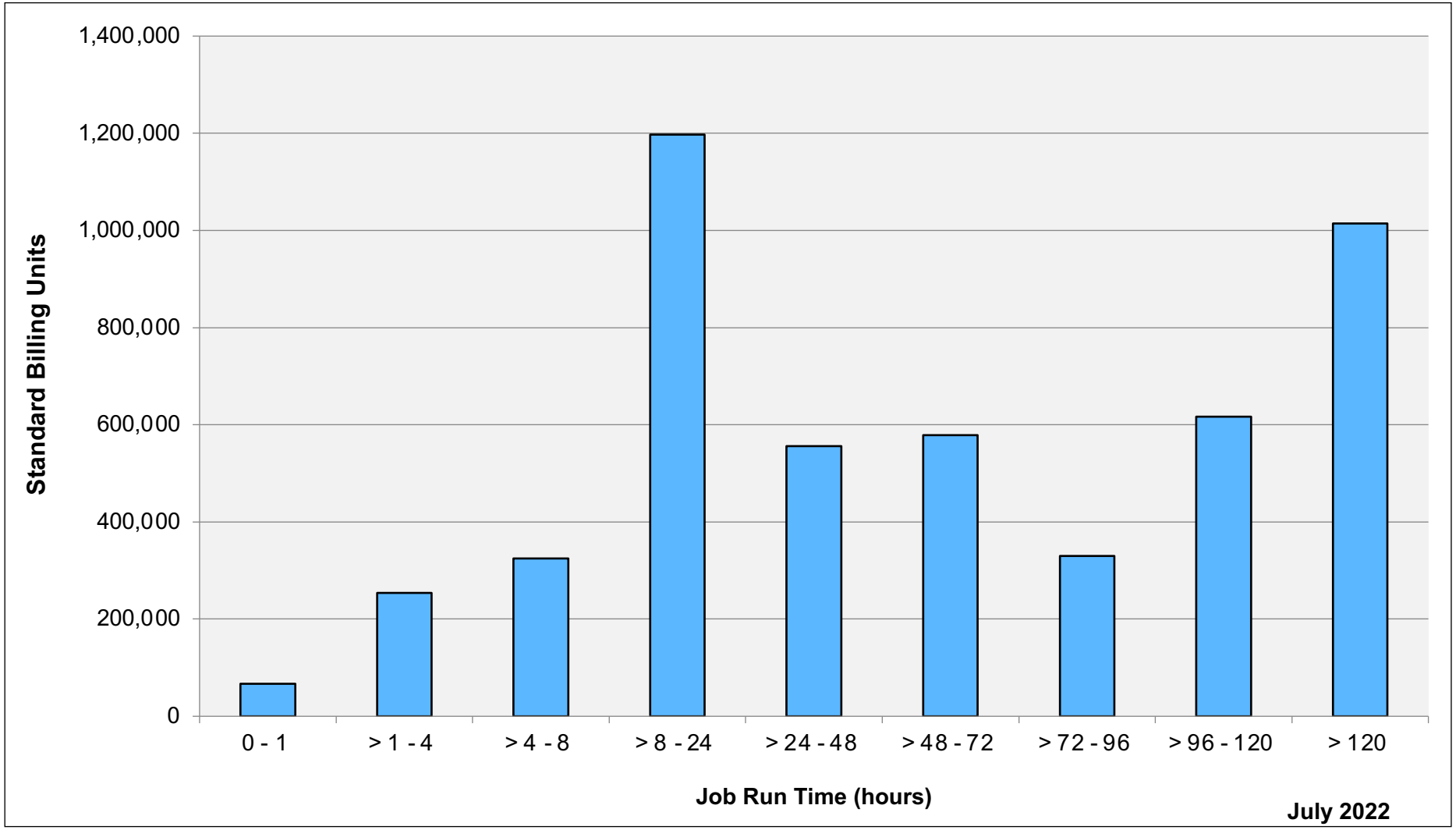
Pleiades: SBUs Reported, Normalized to 30-Day Month



Pleiades: Devel Queue Utilization



Pleiades: Monthly Utilization by Job Length



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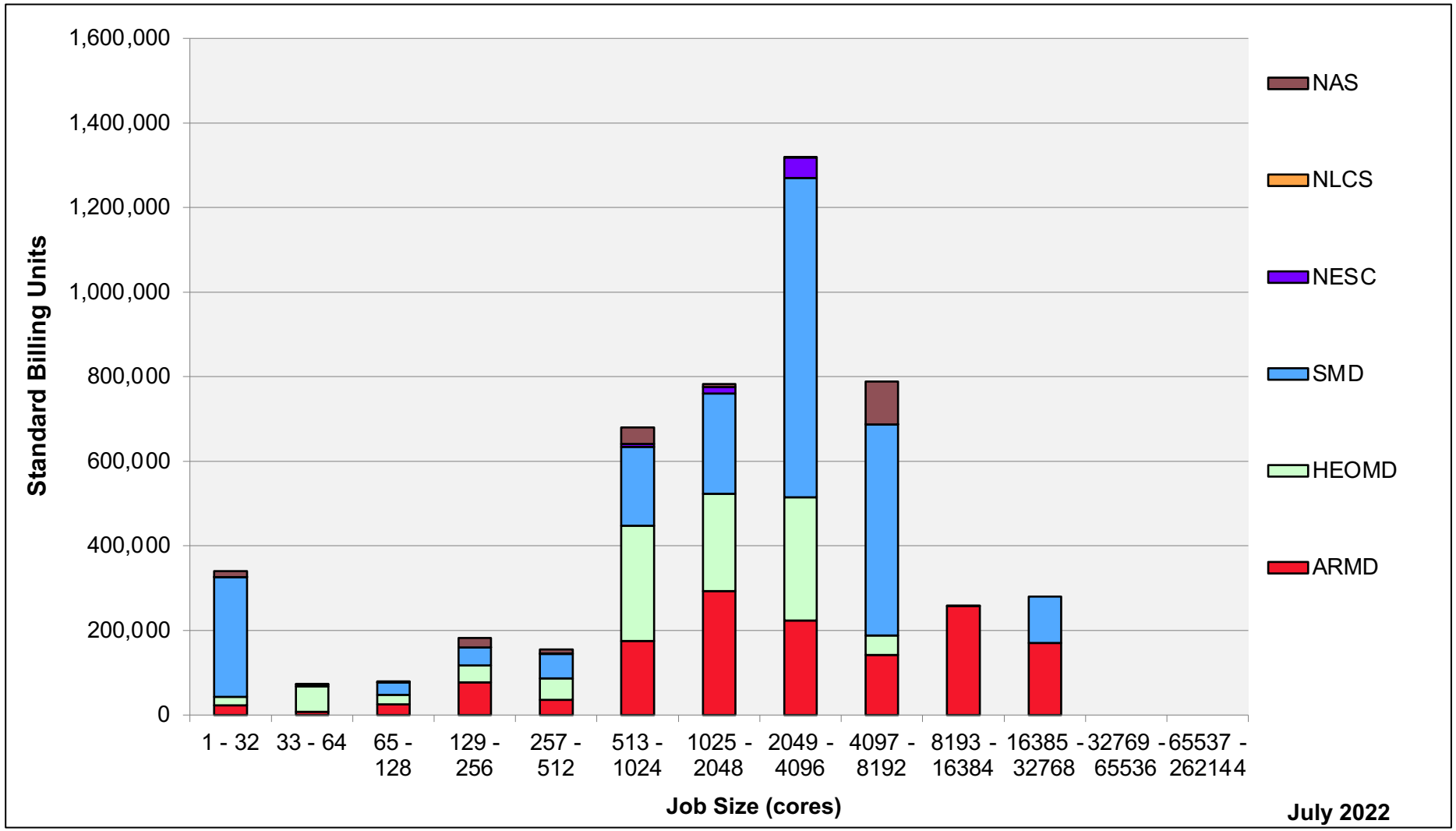

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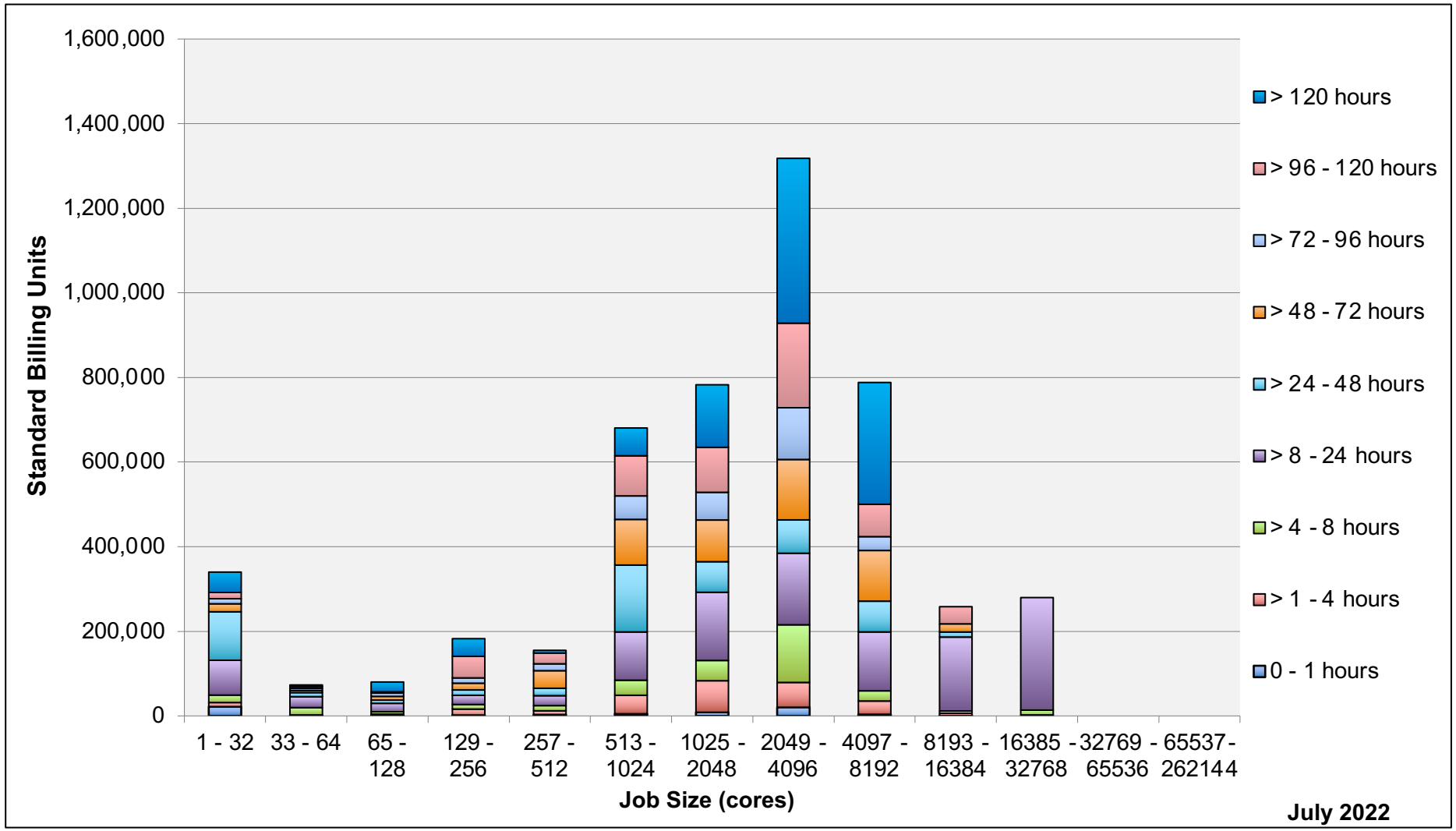
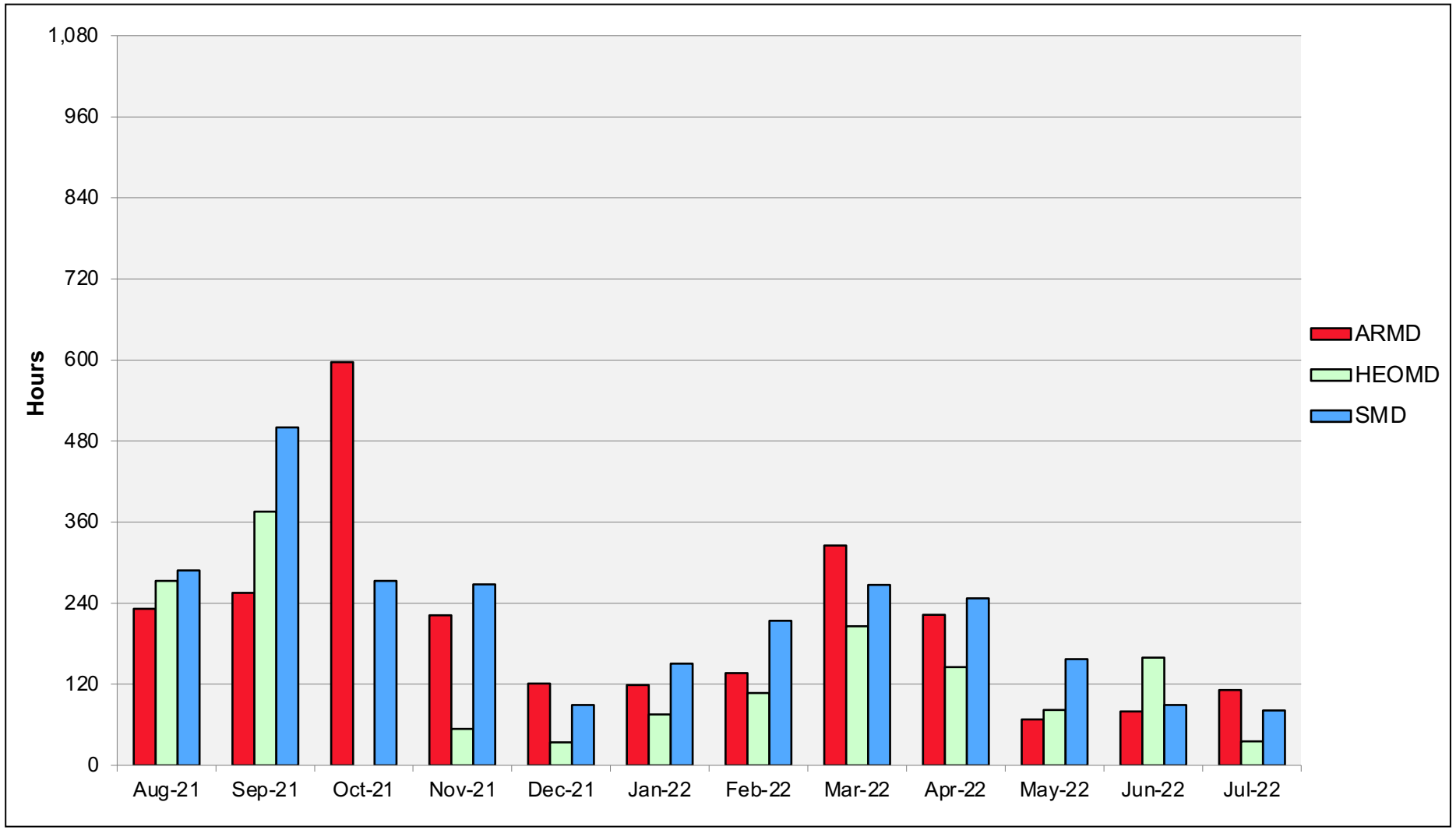
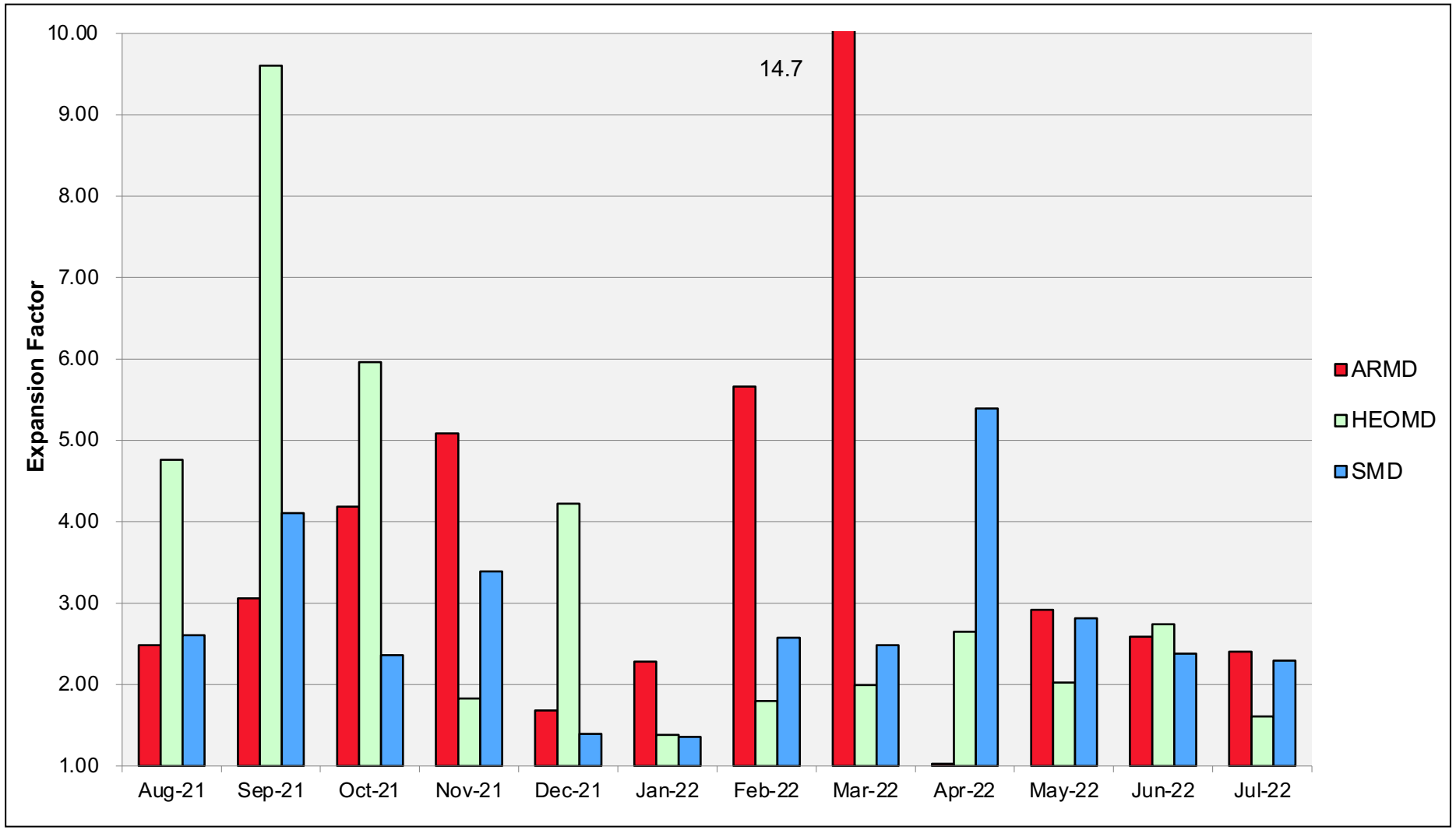


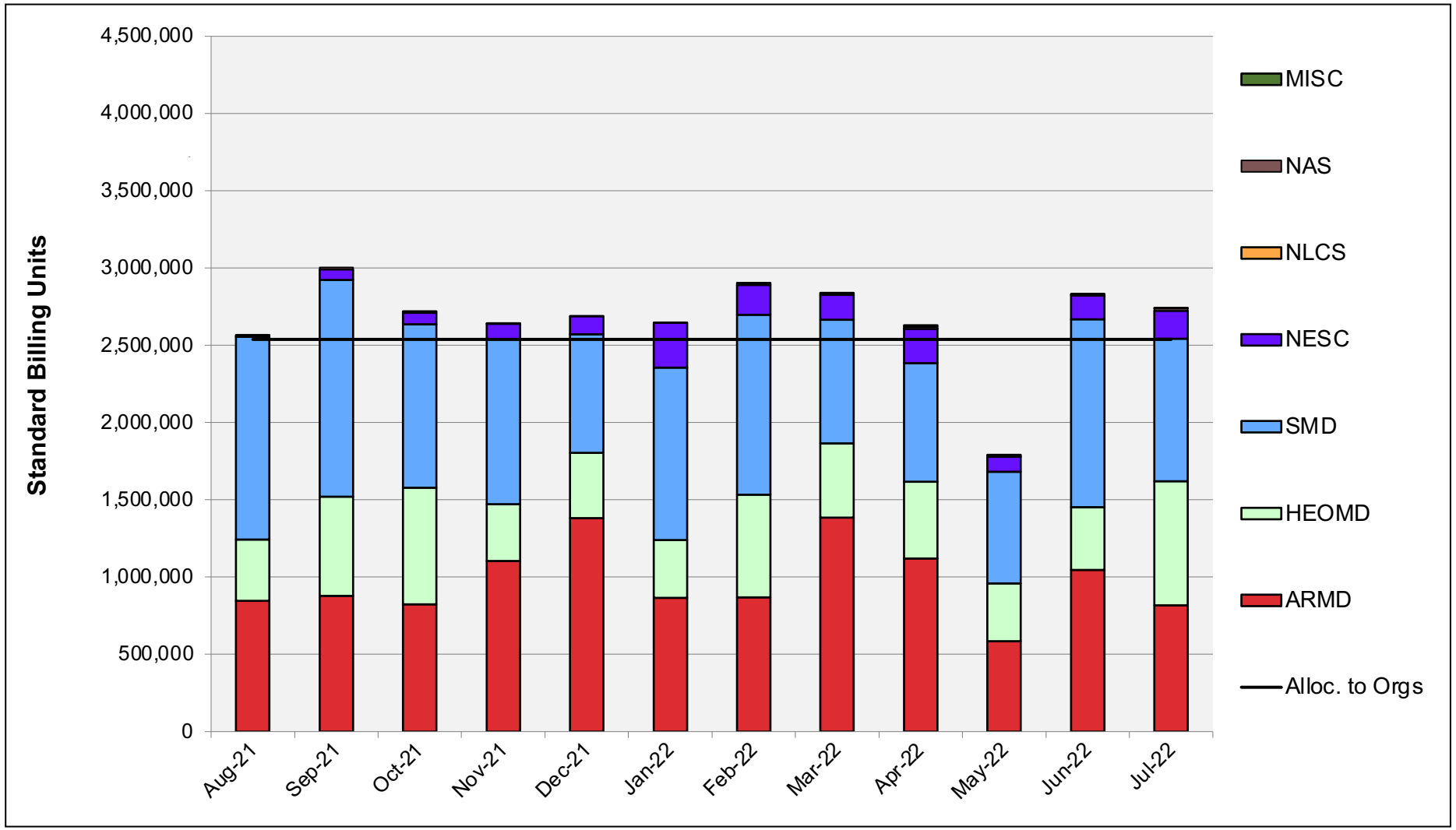
Pleiades: Average Time to Clear All Jobs



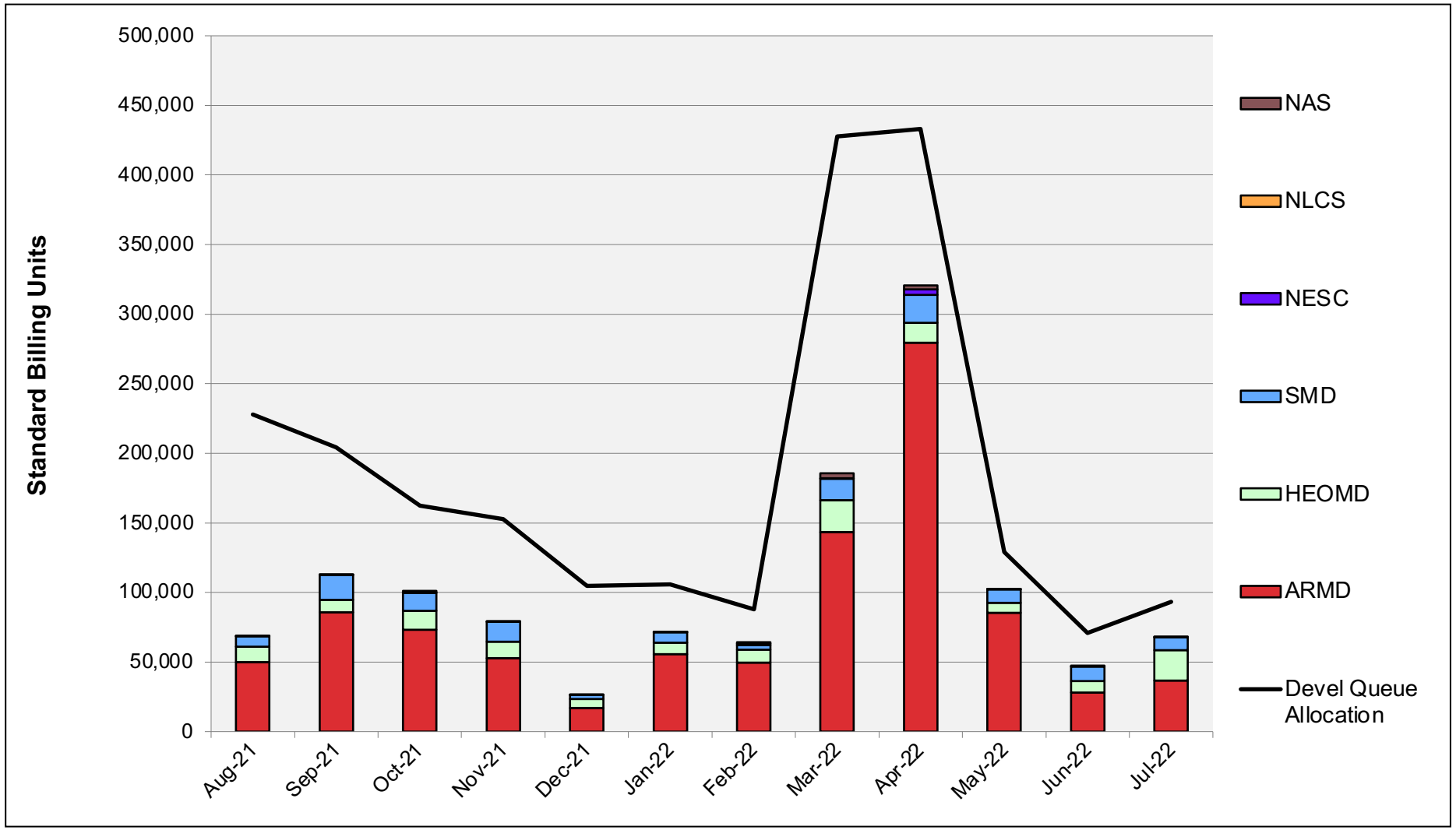
Pleiades: Average Expansion Factor



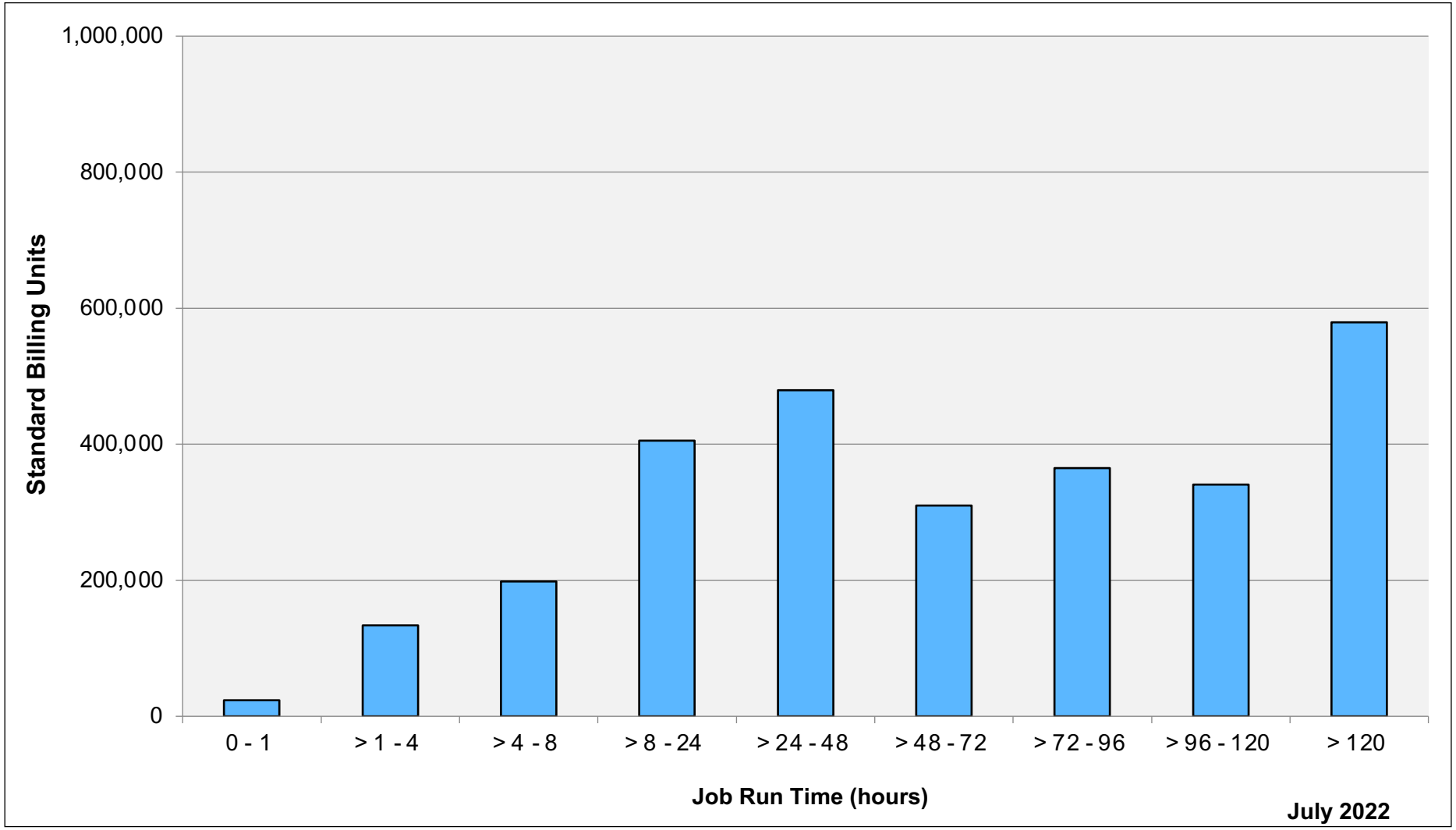
Electra: SBUs Reported, Normalized to 30-Day Month



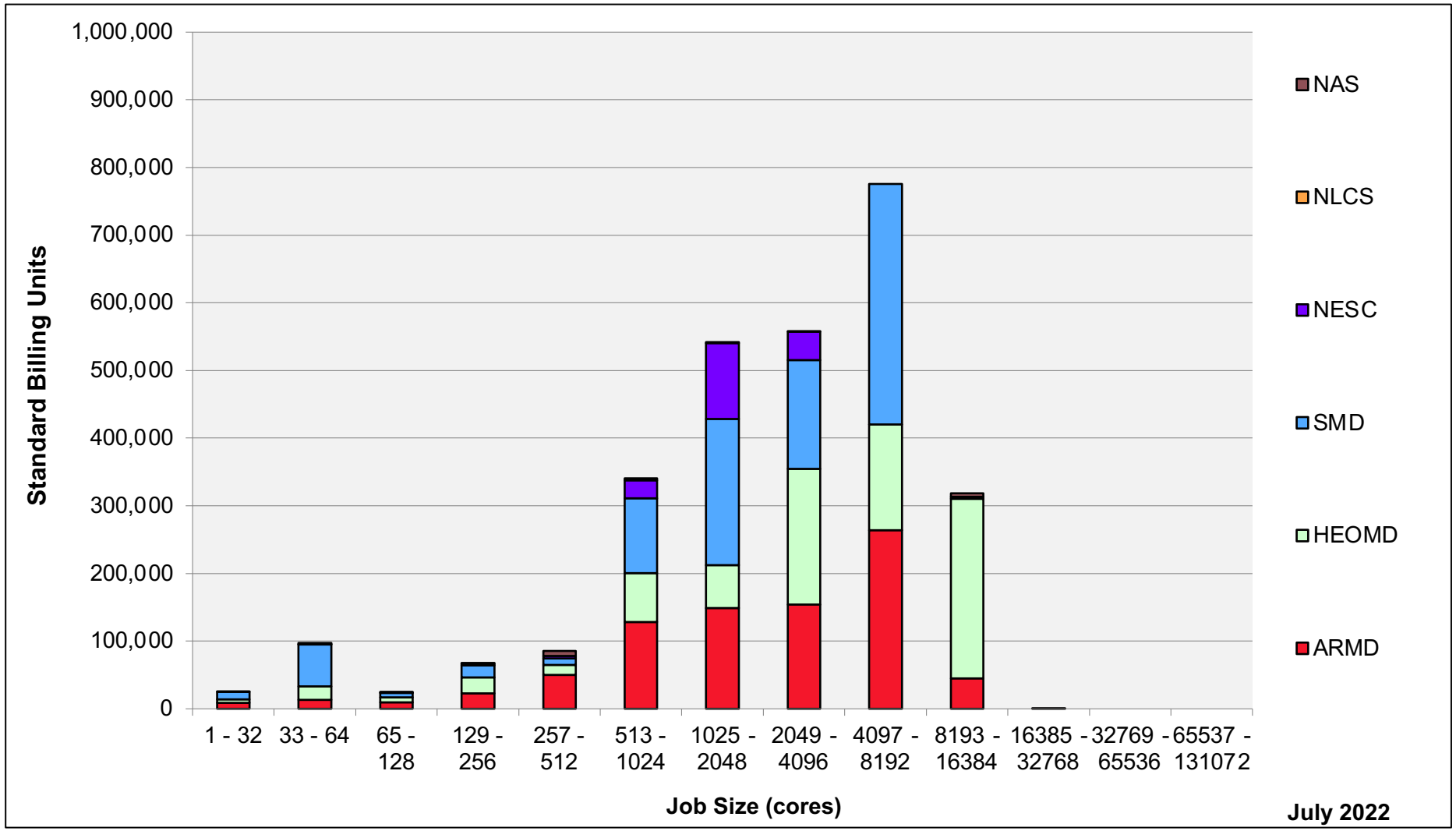
Electra: Devel Queue Utilization



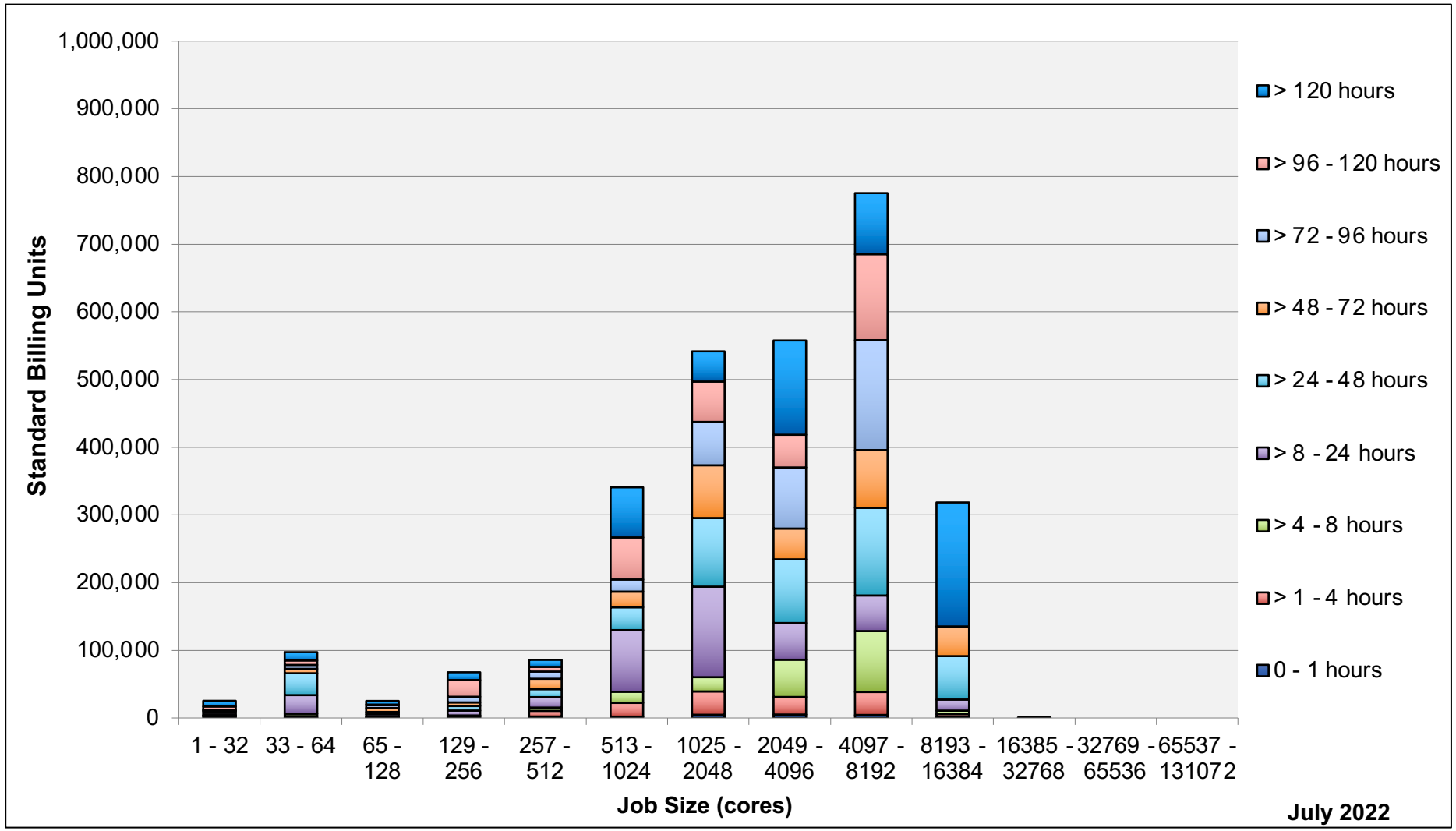
Electra: Monthly Utilization by Job Length



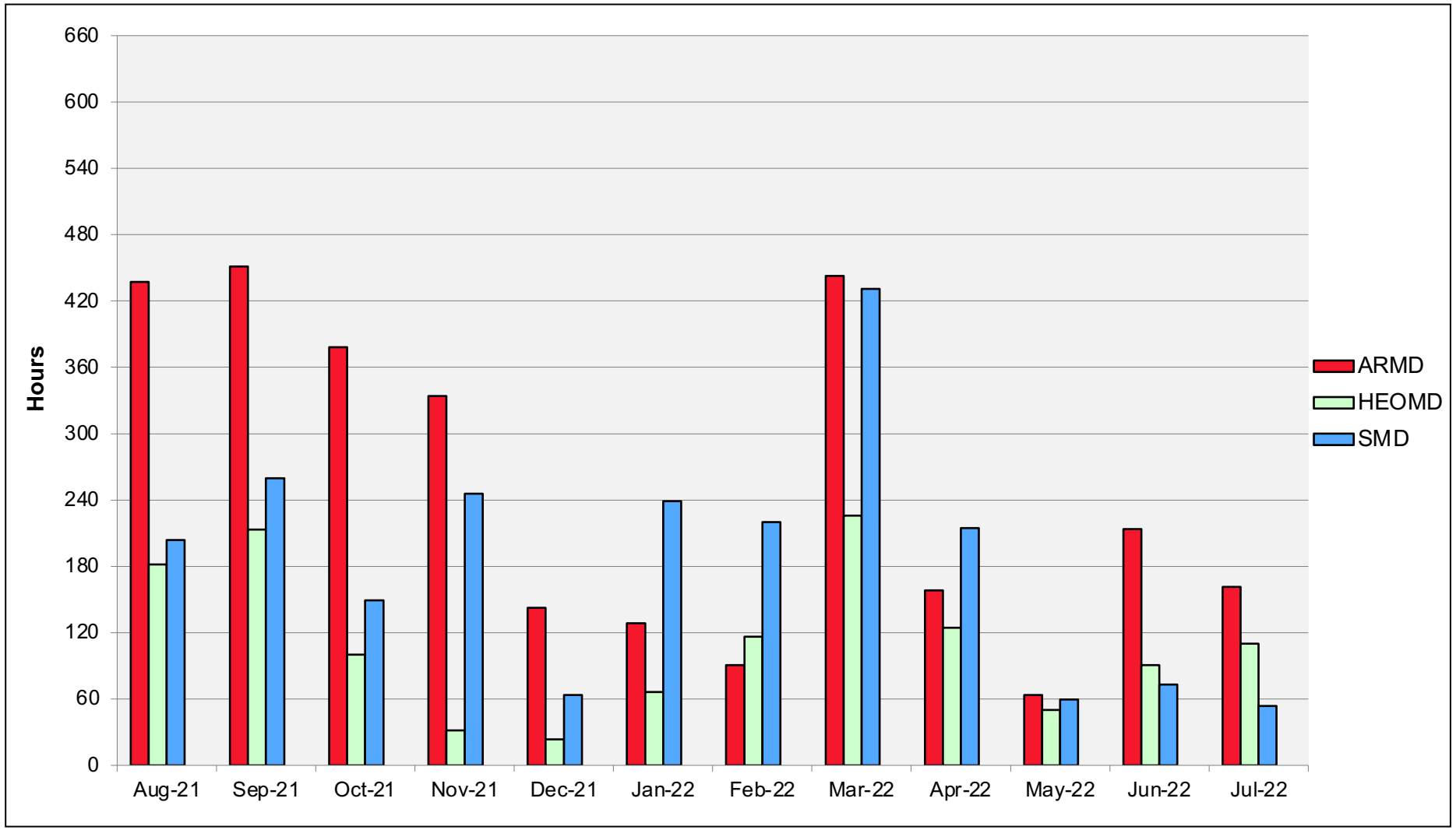
Electra: Monthly Utilization by Job Size



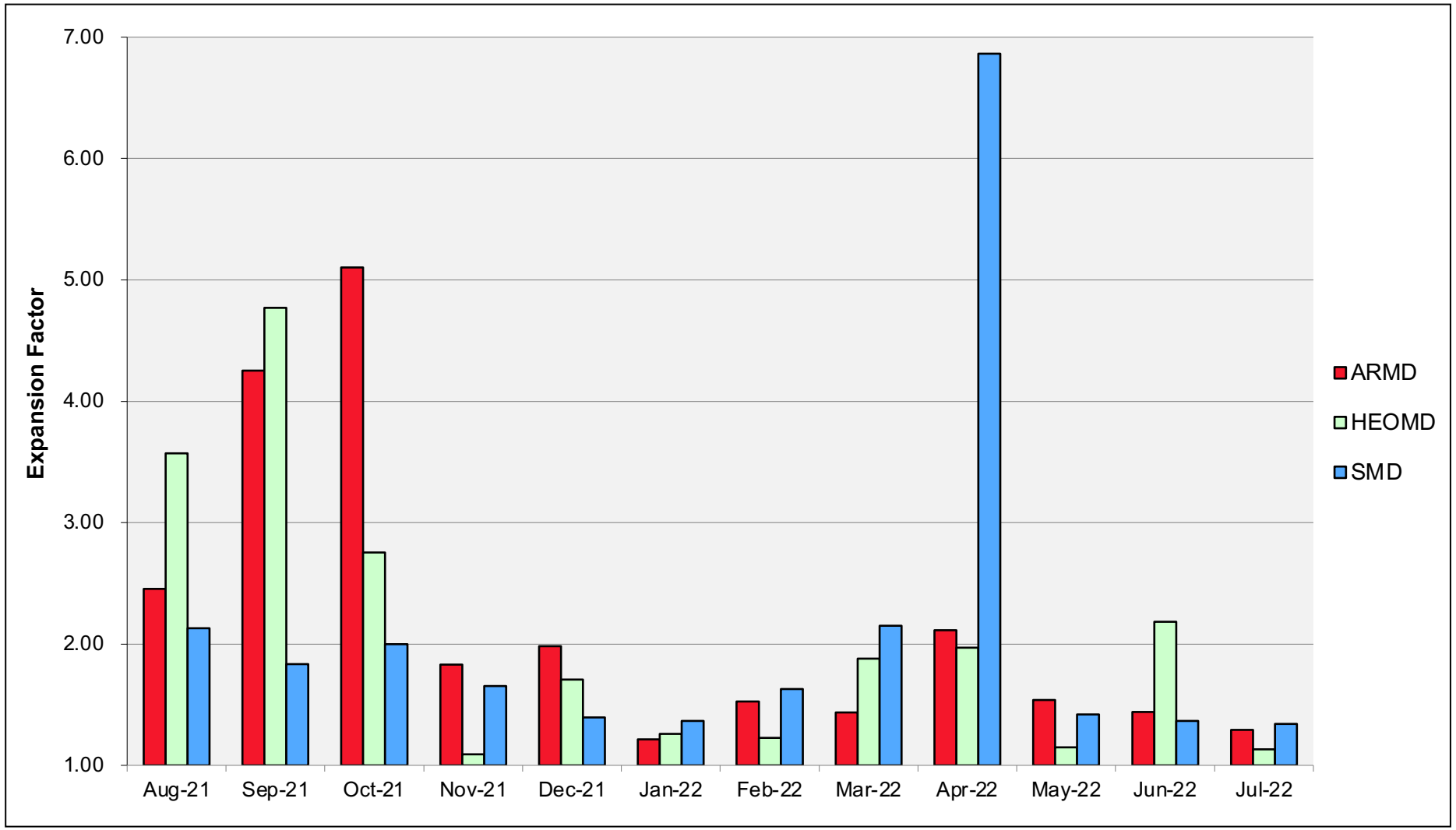
Electra: Monthly Utilization by Size and Length



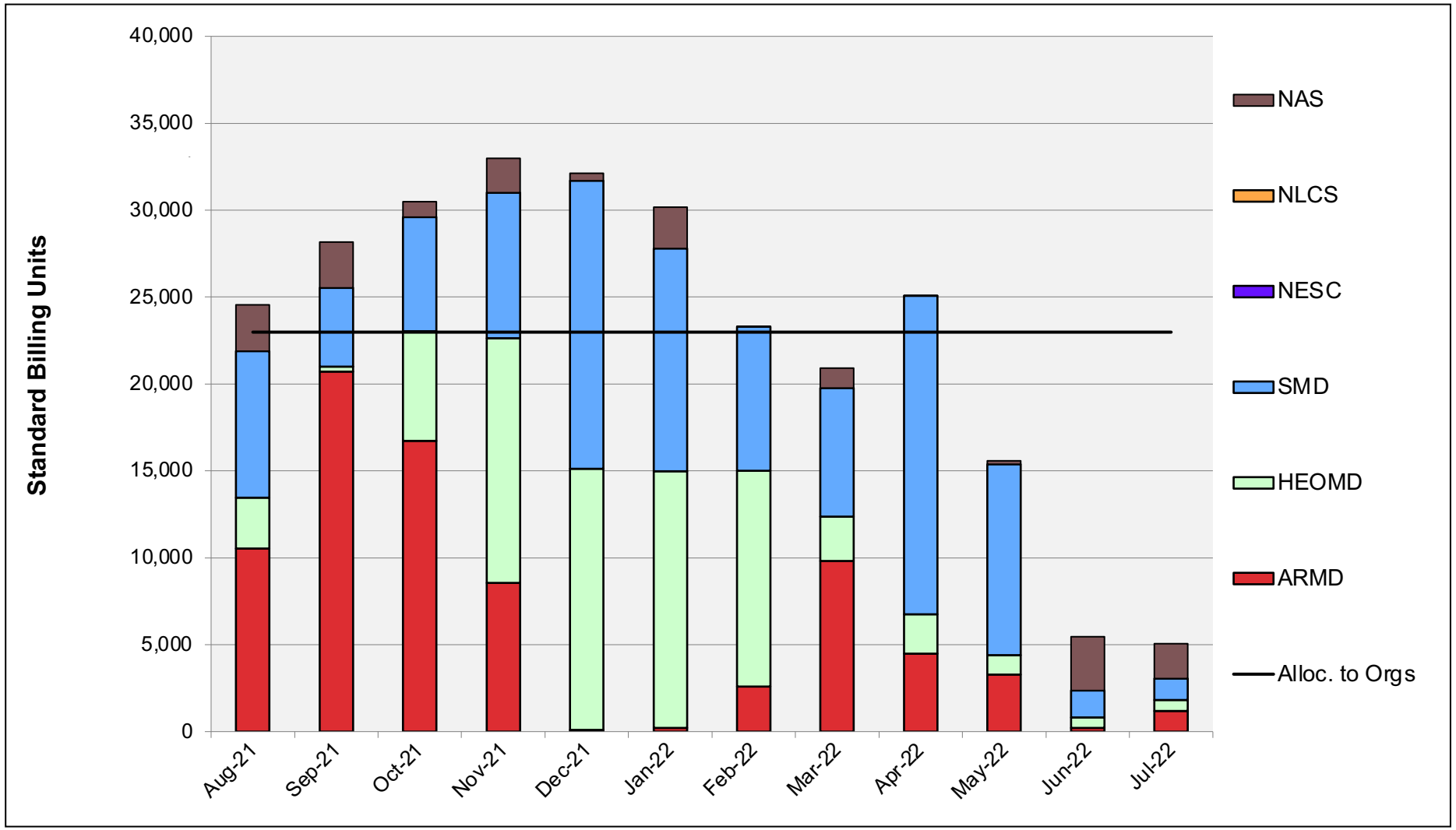
Electra: Average Time to Clear All Jobs



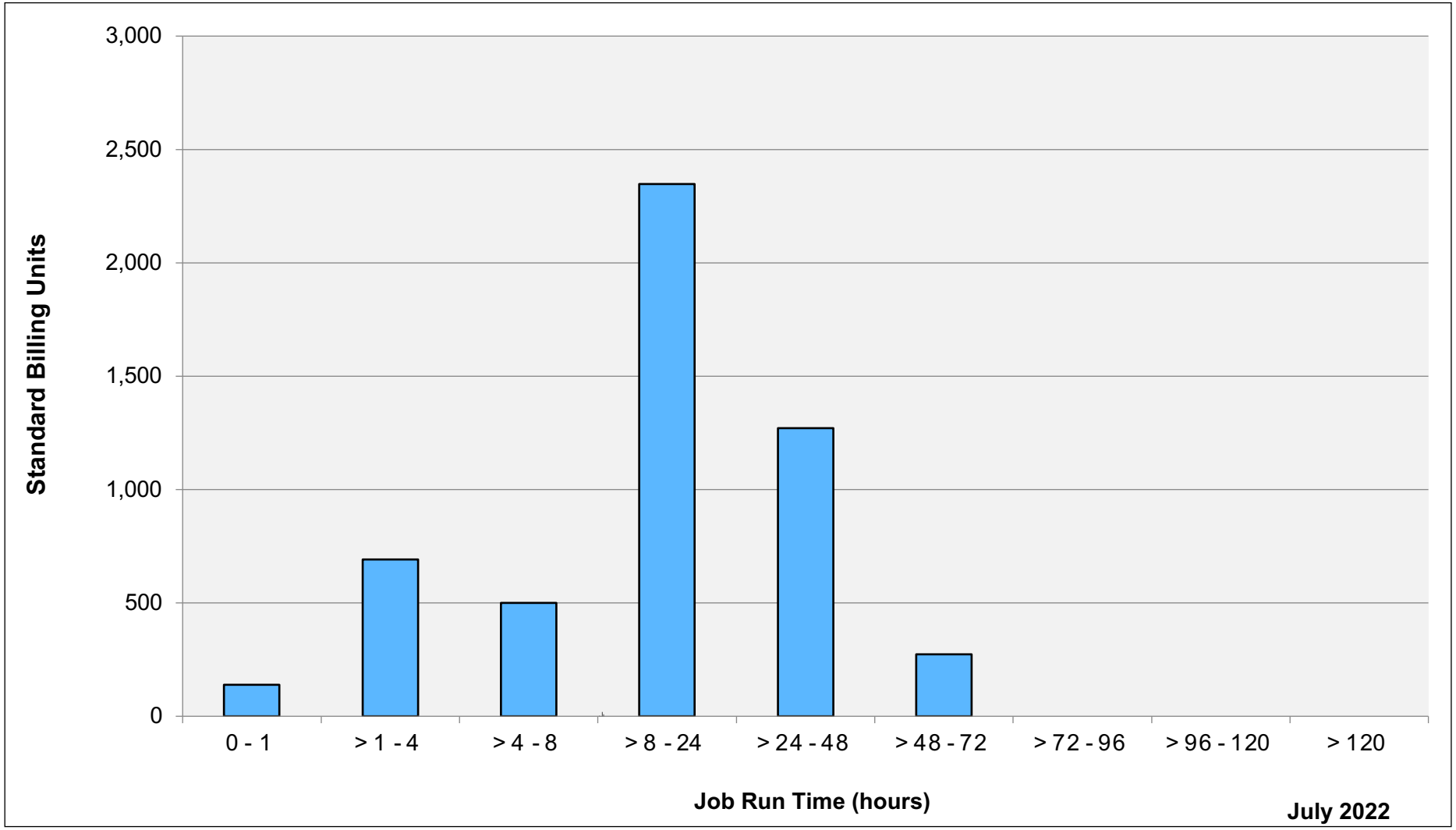
Electra: Average Expansion Factor



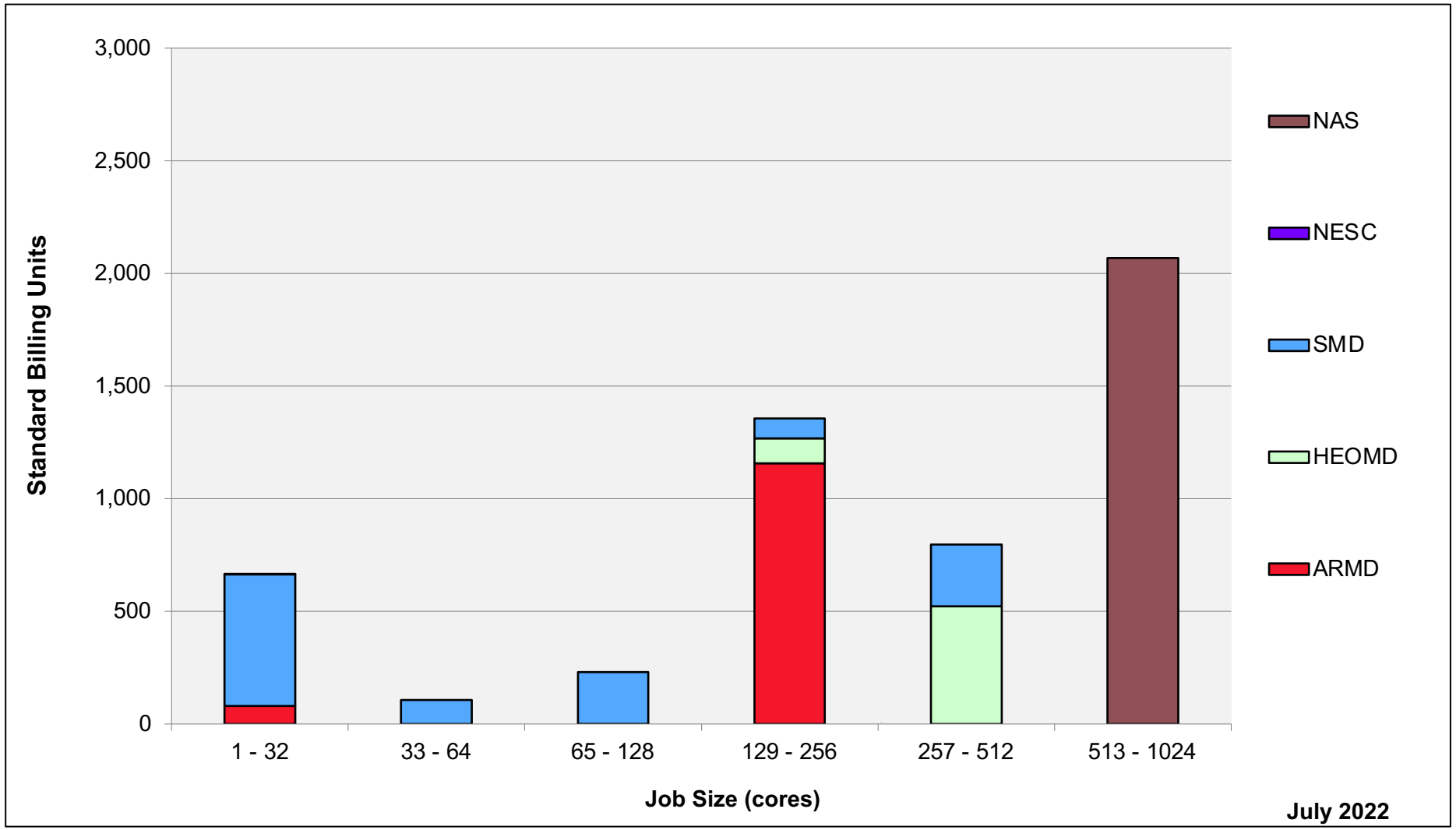
Endeavour: SBUs Reported, Normalized to 30-Day Month



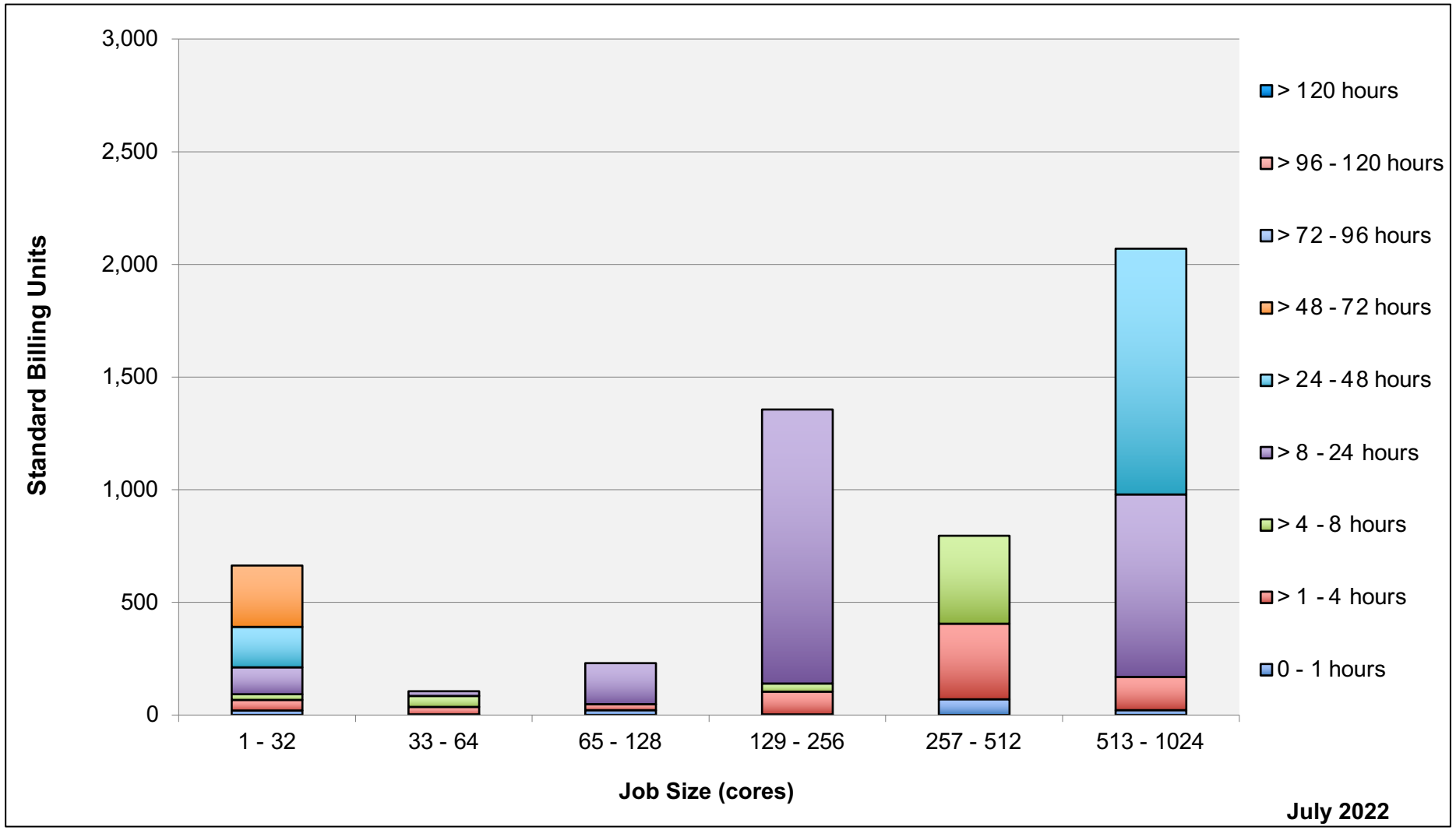
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor